

10556224

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptasxml624

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 APR 02 CAS Registry Number Crossover Limits Increased to
500,000 in Key STN Databases
NEWS 3 APR 02 PATDPAFULL: Application and priority number formats
enhanced
NEWS 4 APR 02 DWPI: New display format ALLSTR available
NEWS 5 APR 02 New Thesaurus Added to Derwent Databases for Smooth
Sailing through U.S. Patent Codes
NEWS 6 APR 02 EMBASE Adds Unique Records from MEDLINE, Expanding
Coverage back to 1948
NEWS 7 APR 07 CA/CAPLUS CLASS Display Streamlined with Removal of
Pre-IPC 8 Data Fields
NEWS 8 APR 07 50,000 World Traditional Medicine (WTM) Patents Now
Available in CAPLUS
NEWS 9 APR 07 MEDLINE Coverage Is Extended Back to 1947
NEWS 10 JUN 16 WPI First View (File WPIFV) will no longer be
available after July 30, 2010
NEWS 11 JUN 18 DWPI: New coverage - French Granted Patents
NEWS 12 JUN 18 CAS and FIZ Karlsruhe announce plans for a new
STN platform
NEWS 13 JUN 18 IPC codes have been added to the INSPEC backfile
(1969-2009)
NEWS 14 JUN 21 Removal of Pre-IPC 8 data fields streamline displays
in CA/CAPLUS, CASREACT, and MARPAT
NEWS 15 JUN 21 Access an additional 1.8 million records exclusively
enhanced with 1.9 million CAS Registry Numbers --
EMBASE Classic on STN
NEWS 16 JUN 28 Introducing "CAS Chemistry Research Report": 40 Years
of Biofuel Research Reveal China Now Atop U.S. in
Patenting and Commercialization of Bioethanol
NEWS 17 JUN 29 Enhanced Batch Search Options in DGENE, USGENE,
and PCTGEN
NEWS 18 JUL 19 Enhancement of citation information in INPADOC
databases provides new, more efficient competitor
analyses

NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
AND CURRENT DISCOVER FILE IS DATED 15 JANUARY 2010.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN customer agreement. This agreement limits use to scientific research. Use for software development or design, implementation of commercial gateways, or use of CAS and STN data in the building of commercial products is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:44:41 ON 22 JUL 2010

=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 15:44:58 ON 22 JUL 2010
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 JUL 2010 HIGHEST RN 1233453-03-6
 DICTIONARY FILE UPDATES: 21 JUL 2010 HIGHEST RN 1233453-03-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

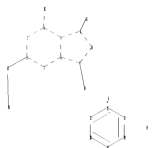
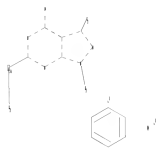
TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>
 Uploading C:\Program Files\Stnexp\Queries\10556224.str



```

chain nodes :
11 12 13 14 15 25
ring nodes :
1 2 3 4 5 6 7 8 9 19 20 21 22 23 24
chain bonds :
2-13 4-12 7-11 9-15 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 19-20 19-24 20-21 21-22 22-23
23-24
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-12 5-6 5-7 6-9 7-8 7-11 8-9 9-15 13-14
exact bonds :
2-13
normalized bonds :
19-20 19-24 20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 :

```

G1:H,CH3

G2:Cb,Ak

G3:[*1],[*2]

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
24:Atom 25:Atom
Generic attributes :
25:
Saturation : Unsaturated

```

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sam
SAMPLE SEARCH INITIATED 15:45:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 604 TO ITERATE

100.0% PROCESSED 604 ITERATIONS 29 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 10606 TO 13554
PROJECTED ANSWERS: 257 TO 903

L2 29 SEA SSS SAM L1

=> s l1 ful
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 191.05 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:45:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11835 TO ITERATE

100.0% PROCESSED 11835 ITERATIONS 579 ANSWERS
SEARCH TIME: 00.00.01

L3 579 SEA SSS FUL L1

=> fil capl
COST IN U.S. DOLLARS SINCE FILE TOTAL
 ENTRY SESSION
FULL ESTIMATED COST 191.54 191.76

FILE 'CAPLUS' ENTERED AT 15:45:49 ON 22 JUL 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching

databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 22 Jul 2010 VOL 153 ISS 4
FILE LAST UPDATED: 21 Jul 2010 (20100721/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

CASplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2010.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 41 L3

=> s l4 not (2010/so or 2009/so or 2008/so or 2007/so or 2006/so or 2005/so)
471899 2010/SO
1018394 2009/SO
1008798 2008/SO
1000575 2007/SO
951525 2006/SO
886676 2005/SO

L5 28 L4 NOT (2010/SO OR 2009/SO OR 2008/SO OR 2007/SO OR 2006/SO OR 2005/SO)

<-----User Break----->

=> d l5 ibib abs hitstr 1-28

L5 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2010:437085 CAPLUS
 DOCUMENT NUMBER: 152:422257
 TITLE: Flavivirus inhibitors and methods for their use
 INVENTOR(S): Padmanabhan, Radhakrishnan; Pattabiraman, Nagarajan;
 Mueller, Niklaus; Nagarajan, Kuppuswamy
 PATENT ASSIGNEE(S): Georgetown University, USA
 SOURCE: PCT Int. Appl., 67pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2010039538	AZ	20100408	WO 2009-US58048	20090923
W:	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PE, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, SE, SI, SK, SM, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

PRIORITY APPLN. INFO.: MARPAT 152:422257 US 2008-99411P P 20080923

OTHER SOURCE(S):

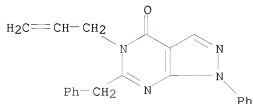
AB Methods of treating, preventing, and/or ameliorating a Flavivirus infection in a subject are disclosed. The methods comprise administering to the subject a therapeutically effective amount of a Flavivirus inhibitor, e.g., a Flavivirus serine protease inhibitor. These methods are useful in treating, preventing, and/or ameliorating Flavivirus infections such as, for example, West Nile Virus, Dengue Virus, and Japanese Encephalitis Virus.

IT 301322-64-5

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (Flavivirus inhibitors and methods for their use in relation to Flavivirus serine protease inhibition)

RN 301322-64-5 CAPLUS

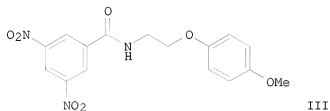
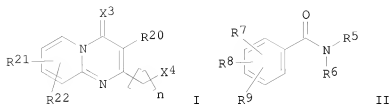
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1,5-dihydro-1-phenyl-6-(phenylmethyl)-5-(2-propen-1-yl)- (CA INDEX NAME)



10556224

L5 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2010:51662 CAPLUS
 DOCUMENT NUMBER: 152:168983
 TITLE: Benzamides, pyridopyrimidines and related compounds as anti-infective compounds and their preparation and use in the treatment of tuberculosis
 INVENTOR(S): Brodin, Priscille; Christophe, Thierry; No, Zaesung; Kim, Jaeseung; Genovesio, Auguste; Fenistein, Denis; Philippe Cedric; Jeon, Heekyoung; Ewann, Fanny Anne; Kang, Sunhee; Lee, Saeyeon; Seo, Min Jung; Park, Eunjung; Contreras Dominguez, Monica; Nam, Ji Youn; Kim, Eun Hye
 PATENT ASSIGNEE(S): Institut Pasteur Korea, S. Korea; Institut National de la Sante et de la Recherche Medicale
 SOURCE: PCT Int. Appl., 328pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2010003533	A2	20100114	WO 2009-EP4379	20090617
W:	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PE, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
PRIORITY APPLN. INFO.:	MARPAT 152:168983		US 2008-132285P	P 20080617
OTHER SOURCE(S):				



AB The invention relates to small mol. compds. of formula I and II and their use in the treatment of bacterial infections, in particular tuberculosis. Compds. of formula I and II wherein n is 0, 1, 2 and 3; X3 is CH2, O, S, and NH; X4 is halo, alkyl, acyloxy, alkoxy, aminoalkoxy, alkyleneoxy, alkylthio, etc.; R20 is acyl, alkoxy, alkyl, alkylamino, etc.; R21 and R22 are independently alkoxy, alkyl, alkylamino, alkylene, alkylthio, etc.; R5 and R6 are independently acyl, alkyl, alkylamino, alkylene, alkylthio, alkynyl, etc.; R7, R8 and R9 are independently alkoxy, alkyl, alkylamino, alkylene, alkylthio, etc.; are claimed. Example compound III was prepared by a general procedure (procedure given). All the invention compds. were evaluated for their antiinfective activity (data given).

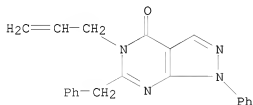
IT 301322-64-5

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of benzamides, pyridopyrimidines and related compds. as antiinfective compds.)

RN 301322-64-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-phenyl-6-(phenylmethyl)-5-(2-propen-1-yl)- (CA INDEX NAME)



L5 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2009:875996 CAPLUS
 DOCUMENT NUMBER: 151:115084
 TITLE: Method using lifespan-altering compounds for altering
 the lifespan of eukaryotic organisms, and screening
 for such compounds
 INVENTOR(S): Goldfarb, David Scott
 PATENT ASSIGNEE(S): University of Rochester, USA
 SOURCE: U.S. Pat. Appl. Publ., 57pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 20
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090163545	A1	20090625	US 2008-341615	20081222
US 20090163545	A1	20090625	US 2008-341615	20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P 20080125
			US 2007-16362P	P 20071221
			US 2008-341615	20081222

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

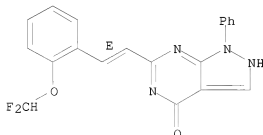
AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 1164488-36-1
 RL: PAC (Pharmacological activity); BIOL (Biological study)
 (method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)

RN 1164488-36-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-[(1E)-2-[2-(difluoromethoxy)phenyl]ethenyl]-1,2-dihydro-1-phenyl- (CA
 INDEX NAME)

Double bond geometry as shown.



L5 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2009:846112 CAPLUS
 DOCUMENT NUMBER: 151:92849
 TITLE: Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds
 INVENTOR(S): Goldfarb, David Scott
 PATENT ASSIGNEE(S): University of Rochester, USA
 SOURCE: U.S. Pat. Appl. Publ., 57pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 20
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090163545	A1	20090625	US 2008-341615	20081222
US 20090163545	A1	20090625	US 2008-341615	20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P 20080125
			US 2007-16362P	P 20071221
			US 2008-341615	20081222

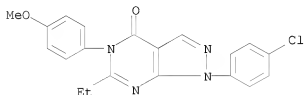
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 901043-30-9
 RL: PAC (Pharmacological activity); BIOL (Biological study)
 (method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)

RN 901043-30-9 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(4-chlorophenyl)-6-ethyl-1,5-dihydro-5-(4-methoxyphenyl)- (CA INDEX NAME)



L5 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2009:846110 CAPLUS
 DOCUMENT NUMBER: 151:92847
 TITLE: Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds
 INVENTOR(S): Goldfarb, David Scott
 PATENT ASSIGNEE(S): University of Rochester, USA
 SOURCE: U.S. Pat. Appl. Publ., 57pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 20
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090163545	A1	20090625	US 2008-341615	20081222
US 20090163545	A1	20090625	US 2008-341615	20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P 20080125
			US 2007-16362P	P 20071221
			US 2008-341615	20081222

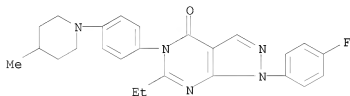
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 901042-68-0
 RL: PAC (Pharmacological activity); BIOL (Biological study)
 (method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)

RN 901042-68-0 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-ethyl-1-(4-fluorophenyl)-1,5-dihydro-5-[4-(4-methyl-1-piperidinyl)phenyl]- (CA INDEX NAME)



L5 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2009:846101 CAPLUS
 DOCUMENT NUMBER: 151:92838
 TITLE: Method using lifespan-altering compounds for altering
 the lifespan of eukaryotic organisms, and screening
 for such compounds
 INVENTOR(S): Goldfarb, David Scott
 PATENT ASSIGNEE(S): University of Rochester, USA
 SOURCE: U.S. Pat. Appl. Publ., 57pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 20
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090163545	A1	20090625	US 2008-341615	20081222
US 20090163545	A1	20090625	US 2008-341615	20081222
PRIORITY APPLN. INFO.:			US 2008-23801P	P 20080125
			US 2007-16362P	P 20071221
			US 2008-341615	20081222

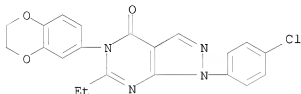
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 901043-60-5
 RL: PAC (Pharmacological activity); BIOL (Biological study)
 (method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)

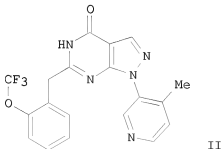
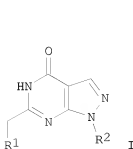
RN 901043-60-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(4-chlorophenyl)-5-(2,3-dihydro-1,4-benzodioxin-6-yl)-6-ethyl-1,5-dihydro- (CA INDEX NAME)



L5 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2009:672279 CAPLUS
 DOCUMENT NUMBER: 151:33617
 TITLE: Preparation of
 1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one derivatives
 as PDE9A modulators for the treatment of CNS disorders
 INVENTOR(S): Eickmeier, Christian; Doerner-Ciossek, Cornelia;
 Fiegen, Dennis; Fox, Thomas; Fuchs, Klaus; Giovannini,
 Riccardo; Heine, Niklas; Hendrix, Martin; Rosenbrock,
 Holger; Schaenzle, Gerhard
 PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany
 SOURCE: PCT Int. Appl., 109pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2009068617	A1	20090604	WO 2008-EP66350	20081127
W:	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
CA 2706018	A1	20090604	CA 2008-2706018	20081127
PRIORITY APPLN. INFO.:			EP 2007-425764	A 20071130
			EP 2008-163548	A 20080903
			EP 2008-169282	A 20081117
			WO 2008-EP66350	W 20081127
OTHER SOURCE(S):		CASREACT 151:33617; MARPAT 151:33617		
GI				



AB The title compds. I [R1 = (un)substituted Ph or pyridyl; R2 = (un)substituted Ph or heteroaryl], useful for the manufacture of medicaments, in particular medicaments for improving perception, concentration, learning and/or memory in patients, were prepared and formulated. Thus, reacting 5-amino-1-(4-methylpyridin-3-yl)-1H-pyrazole-4-carboxamide with Me 2-trifluoromethoxyphenylacetate, afforded 72% II which showed 99% inhibition of PDE9A at 10 μ M.

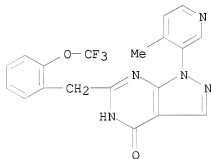
IT	1159677-46-9P	1159677-47-0P	1159677-49-2P
	1159677-50-5P	1159677-51-6P	1159677-52-7P
	1159677-53-8P	1159677-54-9P	1159677-55-0P
	1159677-56-1P	1159677-57-2P	1159677-58-3P
	1159677-59-4P	1159677-60-7P	1159677-61-8P
	1159677-62-9P	1159677-63-0P	1159677-65-2P
	1159677-67-4P	1159677-70-9P	1159677-71-0P
	1159677-73-2P	1159677-75-4P	1159677-76-5P
	1159677-78-7P	1159677-79-8P	1159677-80-1P
	1159677-81-2P	1159677-82-3P	1159677-84-5P
	1159677-85-6P	1159677-86-7P	1159677-87-8P
	1159677-88-9P	1159677-89-0P	1159677-91-4P
	1159677-92-5P	1159677-93-6P	1159677-94-7P
	1159677-96-9P	1159677-97-0P	1159677-98-1P
	1159677-99-2P	1159678-01-9P	

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel 1,5-dihydropyrazolo[3,4-d]pyrimidin-4-ones as PDE9A modulators useful in treatment and prophylaxis CNS disorders)

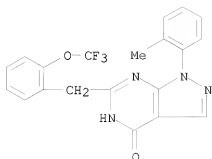
RN 1159677-46-9 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(4-methyl-3-pyridinyl)-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)

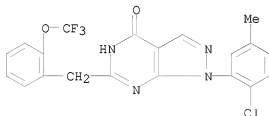


RN 1159677-47-0 CAPLUS

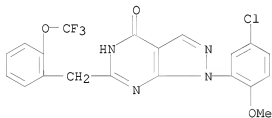
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-methylphenyl)-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



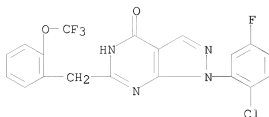
RN 1159677-49-2 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-chloro-5-methoxyphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



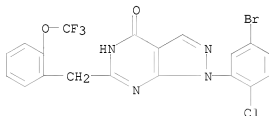
RN 1159677-50-5 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(5-chloro-2-methoxyphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



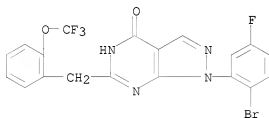
RN 1159677-51-6 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-chloro-5-fluorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



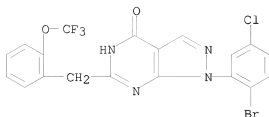
RN 1159677-52-7 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(5-bromo-2-chlorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



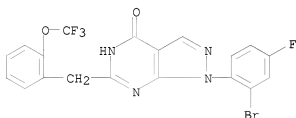
RN 1159677-53-8 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-bromo-5-fluorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



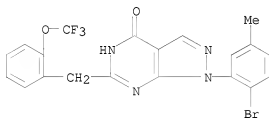
RN 1159677-54-9 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-bromo-5-chlorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



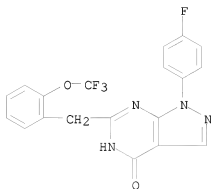
RN 1159677-55-0 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-bromo-4-fluorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



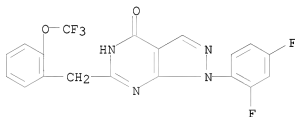
RN 1159677-56-1 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-bromo-5-methylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



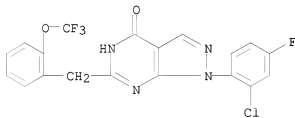
RN 1159677-57-2 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(4-fluorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



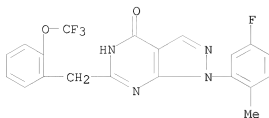
RN 1159677-58-3 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2,4-difluorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]-
 (CA INDEX NAME)



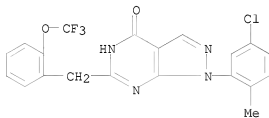
RN 1159677-59-4 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-chloro-4-fluorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



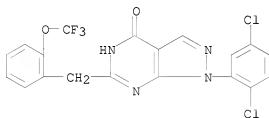
RN 1159677-60-7 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(5-fluoro-2-methylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



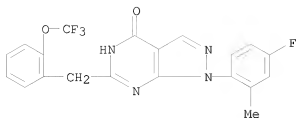
RN 1159677-61-8 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(5-chloro-2-methylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



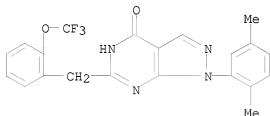
RN 1159677-62-9 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2,5-dichlorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



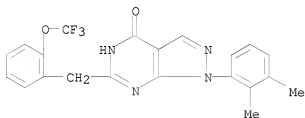
RN 1159677-63-0 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(4-fluoro-2-methylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



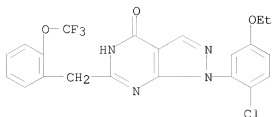
RN 1159677-65-2 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2,5-dimethylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]-
 (CA INDEX NAME)



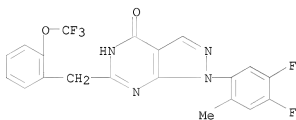
RN 1159677-67-4 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2,3-dimethylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]-
 (CA INDEX NAME)



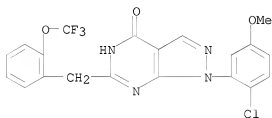
RN 1159677-70-9 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-chloro-5-ethoxyphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



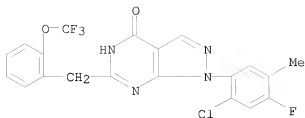
RN 1159677-71-0 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(4,5-difluoro-2-methylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



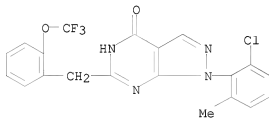
RN 1159677-73-2 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-chloro-5-methoxyphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



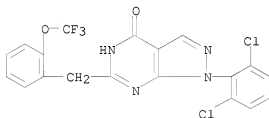
RN 1159677-75-4 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-chloro-4-fluoro-5-methylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



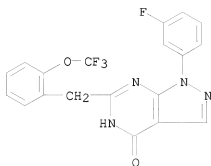
RN 1159677-76-5 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-chloro-6-methylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



RN 1159677-78-7 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2,6-dichlorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)

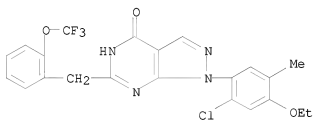


RN 1159677-79-8 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(3,5-dichlorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



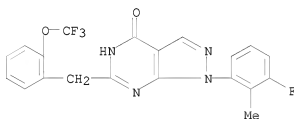
RN 1159677-80-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(2-chloro-4-ethoxy-5-methylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



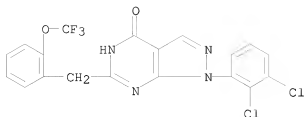
RN 1159677-81-2 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(3-fluoro-2-methylphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)

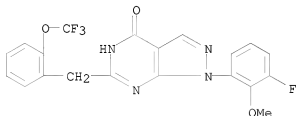


RN 1159677-82-3 CAPLUS

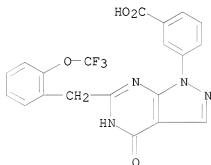
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(2,3-dichlorophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



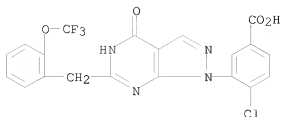
RN 1159677-84-5 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-((3-fluoro-2-methoxyphenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl)methyl]- (CA INDEX NAME)



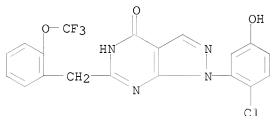
RN 1159677-85-6 CAPLUS
 CN Benzoic acid, 3-[4,5-dihydro-4-oxo-6-[[2-(trifluoromethoxy)phenyl)methyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]- (CA INDEX NAME)



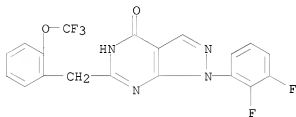
RN 1159677-86-7 CAPLUS
 CN Benzoic acid, 4-chloro-3-[4,5-dihydro-4-oxo-6-[[2-(trifluoromethoxy)phenyl)methyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]- (CA INDEX NAME)



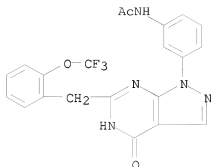
RN 1159677-87-8 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-((2-chloro-5-(trifluoromethoxy)phenyl)methyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl)methyl]- (CA INDEX NAME)



RN 1159677-88-9 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-((2-chloro-5-(trifluoromethoxy)phenyl)methyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl)methyl]- (CA INDEX NAME)

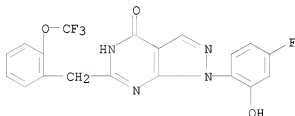


RN 1159677-89-0 CAPLUS
 CN Acetamide, N-[3-[4,5-dihydro-4-oxo-6-[[2-(trifluoromethoxy)phenyl)methyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl]phenyl]- (CA INDEX NAME)



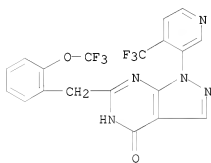
RN 1159677-91-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(4-fluoro-2-hydroxyphenyl)-1,5-dihydro-6-([2-
(trifluoromethoxy)phenyl]methyl)- (CA INDEX NAME)



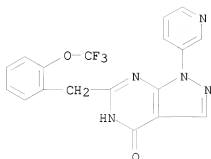
RN 1159677-92-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-([2-(trifluoromethoxy)phenyl]methyl)-1-[4-(trifluoromethyl)-
3-pyridinyl]- (CA INDEX NAME)

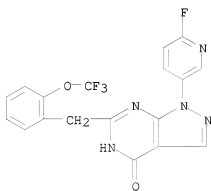


RN 1159677-93-6 CAPLUS

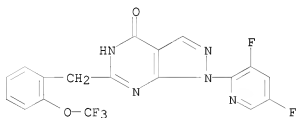
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(3-pyridinyl)-6-([2-(trifluoromethoxy)phenyl]methyl)- (CA
INDEX NAME)



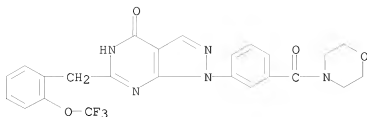
RN 1159677-94-7 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-((6-fluoro-3-pyridinyl)-1,5-dihydro-6-[[2-
 (trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



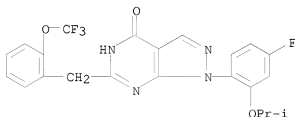
RN 1159677-96-9 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-((3,5-difluoro-2-pyridinyl)-1,5-dihydro-6-[[2-
 (trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



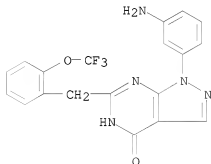
RN 1159677-97-0 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-([2-chloro-5-(1-piperidinylcarbonyl)phenyl]-1,5-dihydro-6-[[2-
 (trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



IT 1159679-06-7P 1159679-09-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of novel 1,5-dihydropyrazolo[3,4-d]pyrimidin-4-ones as PDE9A
 modulators useful in treatment and prophylaxis CNS disorders)
 RN 1159679-06-7 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-[4-fluoro-2-(1-methylethoxy)phenyl]-1,5-dihydro-6-[[2-
 (trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



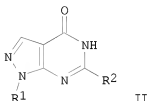
RN 1159679-09-0 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(3-aminophenyl)-1,5-dihydro-6-[[2-(trifluoromethoxy)phenyl]methyl]- (CA
 INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2009:404853 CAPLUS
 DOCUMENT NUMBER: 150:423209
 TITLE: Method for preparation of pyrazole[3,4-d]pyrimidinone
 INVENTOR(S): Zhong, Ping; Lin, Qiulian; Tang, Riyuan; Luo, Yi; Luo, Peisong
 PATENT ASSIGNEE(S): Wenzhou University, Peop. Rep. China
 SOURCE: Faming Zhuanli Shengqing Gongkai Shuomingshu, 7pp.
 CODEN: CNXXEV
 DOCUMENT TYPE: Patent
 LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

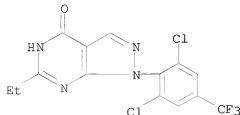
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101397299	A	20090401	CN 2007-10181063	20070929
PRIORITY APPLN. INFO.:			CN 2007-10181063	20070929
OTHER SOURCE(S):			CASREACT 150:423209; MARPAT 150:423209	
GI				



AB The claimed pyrazole[3,4-d]pyrimidinone I (R2 = H, Me, Et) was prepared from 5-amino-4-cyano-pyrazole II (R1 = H, alkyl, or aryl) and carboxylic acid in the presence of POCl3 as catalyst via cyclocondensation in one step to provide the title product. This method has simple operation, moderate condition, short reaction time, convenient post treatment, and high yield.

IT 1142408-68-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of pyrazolepyrimidinone by cyclocondensation of aminocyanopyrazole and carboxylic acid)

RN 1142408-68-1 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-6-ethyl-1,5-dihydro- (CA INDEX NAME)

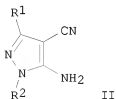
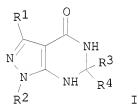


10556224

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L5 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2008:720343 CAPLUS
 DOCUMENT NUMBER: 149:128843
 TITLE: Novel method for synthesizing
 pyrazolo[3,4-d]pyrimidin-4(5H)-one derivative from
 3-amino-4-cyano-1H-pyrazole derivative
 INVENTOR(S): Li, Jiarong; Zhang, Lijun; Shi, Daxin; Wang, Chunxia;
 Li, Qing; Wang, Dong; Zhang, Qi; Zhang, Ling; Fan,
 Yanqiu
 PATENT ASSIGNEE(S): Beijing Institute of Technology, Peop. Rep. China
 SOURCE: Faming Zhuanli Shengqing Gongkai Shuomingshu, 10pp.
 CODEN: CNXXEV
 DOCUMENT TYPE: Patent
 LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
CN 101195626	A	20080611	CN 2007-10304271	20071226
PRIORITY APPLN. INFO.:			CN 2007-10304271	20071226
OTHER SOURCE(S):		CASREACT 149:128843; MARPAT 149:128843		
GI				

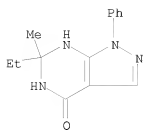


AB The title pyrazolo[3,4-d]pyrimidin-4(5H)-one derivative I (wherein, R1 and/or R2 = aryl, alkyl, halo, NO2, NO, or alkoxy; and R3 and/or R4 = alkyl, cycloalkyl, or arylalkyl) is prepared by the reaction of 3-amino-4-cyano-1H-pyrazole derivative II with ketone R3COR4 in the presence of catalyst under conventional heating and purified by crystallization or column chromatog. The catalyst is Lewis acid, Bronsted acid, or base, preferably ZnCl2, AlCl3, CuCl2, CuCl, HCl, H2SO4, pyridine, piperidine, Na2CO3, NaOH, KOH, Na alkoxide, or K alkoxide. The inventive method has the advantages of easily-available raw materials, simple process, mild reaction condition, and wide applicable range.

IT 1035893-75-4P
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of pyrazolopyrimidinone by reaction of 3-amino-4-cyanopyrazole with ketone in presence of Lewis acid, Bronsted acid, or base)

RN 1035893-75-4 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-ethyl-1,5,6,7-tetrahydro-6-methyl-1-phenyl- (CA INDEX NAME)

10556224



L5 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2008:256115 CAPLUS

DOCUMENT NUMBER: 148:285203

TITLE: Benzene, pyridine, and pyridazine derivatives as
HSP-90 inhibitors and their preparation,
pharmaceutical compositions and use in the treatment
of proliferative diseases

INVENTOR(S): Huang, Kenneth He; Mangette, John; Barta, Thomas;
Hughes, Philip; Hall, Steven E.; Veal, James

PATENT ASSIGNEE(S): Serenex, Inc., USA

SOURCE: PCT Int. Appl., 432 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

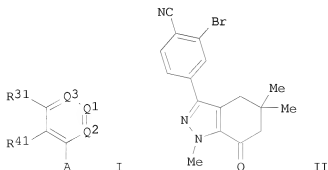
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008024978	A2	20080228	WO 2007-US76770	20070824
WO 2008024978	A3	20080821		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
US 20080119457	A1	20080522	US 2007-844816	20070824
PRIORITY APPLN. INFO.:			US 2006-823414P	P 20060824

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 148:285203

GI



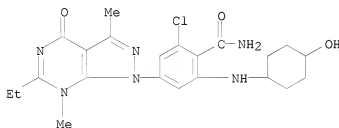
AB Disclosed are compds. and pharmaceutically acceptable salts of formula I. Compds. of formula I are useful in the treatment of diseases and/or conditions related to cell proliferation, such as cancer, inflammation, arthritis, angiogenesis, or the like. Also disclosed are pharmaceutical compns. comprising compds. of the invention and methods of treating the aforementioned conditions using such compds. Compds. of formula I wherein Q1, Q2 and Q3 are independently N and CRx, provided that no more than two of Q1, Q2 and Q3 are N; each Rx is independently H, halo, (hetero)aryl, C1-6 (halo)alkyl, etc.; A is (un)substituted (hetero)bicyclic derivative and (un)substituted 5-membered (hetero)cyclic ring; R31 and R41 are independently H, halo, C1-15 (hetero)alkyl, etc.; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by epoxidn. of 4,4-dimethylcyclohex-2-enone; the resulting 5,5-dimethyl-7-oxabicyclo[4.1.0]heptan-2-one underwent addition of methanol followed by elimination to give 2-methoxy-4,4-dimethylcyclohex-2-enone, which underwent acylation with 3-bromo-4-cyanobenzoyl chloride to give 2-bromo-4-(3-methoxy-5,5-dimethyl-2-oxocyclohex-3-enecarbonyl)benzonitrile, which underwent cyclization with methylhydrazine to give compound II. All the invention compds. were evaluated for their HSP-90 inhibitory activity (some data given).

IT 1017860-58-OP 1017864-43-5P 1017869-67-8P
1017872-72-8P

RL: PAC (Pharmacological activity); PRPH (Prophetic); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prophetic drug candidate; preparation of benzene, pyridine, and pyridazine derivs. as HSP-90 inhibitors useful in the treatment of proliferative diseases)

RN 1017860-58-0 CAPLUS

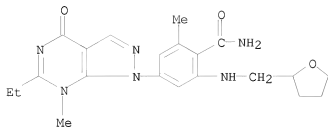
CN Benzamide, 2-chloro-4-(6-ethyl-4,7-dihydro-3,7-dimethyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)-6-[(4-hydroxycyclohexyl)amino]- (CA INDEX NAME)



RN 1017864-43-5 CAPLUS

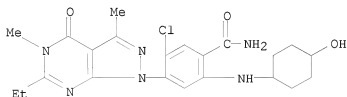
CN Benzamide, 4-(6-ethyl-4,7-dihydro-7-methyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)-2-methyl-6-[(tetrahydro-2-furanyl)methyl]amino]- (CA INDEX NAME)

10556224



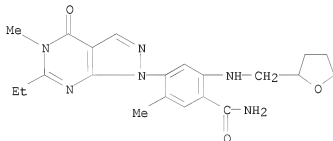
RN 1017869-67-8 CAPLUS

CN Benzamide, 5-chloro-4-(6-ethyl-4,5-dihydro-3,5-dimethyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)-2-[(4-hydroxycyclohexyl)amino]- (CA INDEX NAME)



RN 1017872-72-8 CAPLUS

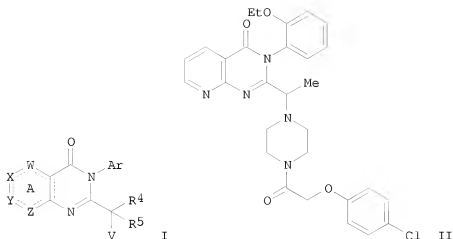
CN Benzamide, 4-(6-ethyl-4,5-dihydro-5-methyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)-5-methyl-2-[(tetrahydro-2-furanyl)methylamino]- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L5 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2007:729227 CAPLUS
 DOCUMENT NUMBER: 147:143456
 TITLE: Fused pyrimidones and thiopyrimidones, and their
 preparation, pharmaceutical compositions and use in
 killing or reducing cancer cell proliferation
 INVENTOR(S): Venkat, Raj Gopal; Qi, Longwu; Pierce, Michael;
 Robbins, Paul B.; Sahasrabudhe, Sudhir R.; Selliah,
 Robert
 PATENT ASSIGNEE(S): Prolexys Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 77 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007076085	A2	20070705	WO 2006-US49168	20061222
WO 2007076085	A3	20070823		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			
US 20090170834	A1	20090702	US 2009-86909	20090109
PRIORITY APPLN. INFO.:			US 2005-753916P	P 20051222
			US 2006-834989P	P 20060727
			WO 2006-US49168	W 20061222
OTHER SOURCE(S):	CASREACT 147:143456; MARPAT 147:143456			
GI				



AB Comps. represented by structural formula I: are useful, for example, in the effective killing or reduction in rate of proliferation of cancer cells, such as in patients suffering from cancer. In addition to the comps. themselves, the invention provides pharmaceutical comps. of the comps. and method of treatment using the comps. Comps. of formula I wherein ring A is optionally substituted: W is absent, C, N, S and O; X, Y and Z is C, N, S and O where at least one of X, Y and Z is N if W is C; Ar is (un)substituted phenyl; R⁴ and R⁵ are independently H, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted heterocyclyl, and (un)substituted aryl; V is substituted amine and cyclic amines; dotted lines are single and double bonds; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by a general procedure. All the invention comps. were evaluated for their ability to kill or reduce cancer cell proliferation.

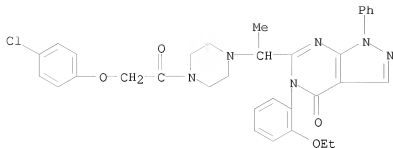
IT 943431-00-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

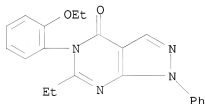
(drug candidate; preparation of fused pyrimidine and thiopyrimidine comps. useful in killing or reducing cancer cell proliferation)

RN 943431-00-3 CAPLUS

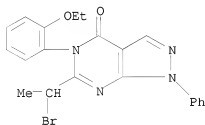
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[1-[4-[2-(4-chlorophenoxy)acetyl]-1-piperazinyl]ethyl]-5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl- (CA INDEX NAME)



IT 943431-16-1P 943431-17-2P 943431-18-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (intermediate; preparation of fused pyrimidone and thiopyrimidone compds.
 useful in killing or reducing cancer cell proliferation)
 RN 943431-16-1 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 5-(2-ethoxyphenyl)-6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)

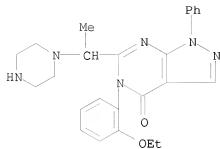


RN 943431-17-2 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(1-bromoethyl)-5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl- (CA INDEX NAME)



RN 943431-18-3 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl-6-[1-(1-piperazinyl)ethyl]- (CA
 INDEX NAME)

10556224



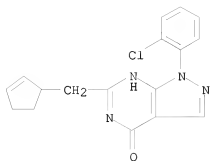
OS.CITING REF COUNT: 3

THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L5 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2006:1253041 CAPLUS
 DOCUMENT NUMBER: 146:757
 TITLE: Use of pyrazolopyrimidine compounds for the treatment
 of cardiovascular diseases
 INVENTOR(S): Hendrix, Martin; Wunder, Frank; Tersteegen, Adrian;
 Stasch, Johannes-Peter
 PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany
 SOURCE: PCT Int. Appl., 48pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006125548	A1	20061130	WO 2006-EP4591	20060516
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
DE 102005024493	A1	20061130	DE 2005-102005024493	20050527
EP 1888076	A1	20080220	EP 2006-753634	20060516
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR			
PRIORITY APPLN. INFO.:			DE 2005-102005024493A	20050527
			WO 2006-EP4591	W 20060516
OTHER SOURCE(S):	MARPAT 146:757			
AB	The invention discloses the use of pyrazolopyrimidine compds. for producing medicaments drugs for treating cardiovascular diseases.			
IT	794568-65-3 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pyrazolopyrimidine compds. for treatment of cardiovascular diseases)			
RN	794568-65-3 CAPLUS			
CN	4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro- (CA INDEX NAME)			

10556224



REFERENCE COUNT:

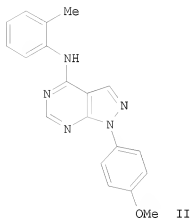
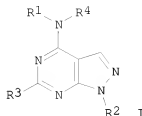
9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2006:471917 CAPLUS
 DOCUMENT NUMBER: 144:488675
 TITLE: Preparation of 1,4-substituted pyrazolopyrimidines as
 kinase inhibitors, particularly EphB4 inhibitors
 INVENTOR(S): Schmiedeberg, Niko; Furet, Pascal; Imbach, Patricia;
 Holzer, Philipp
 PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma GmbH
 SOURCE: PCT Int. Appl., 88 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

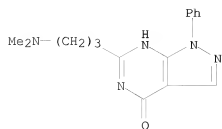
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006050946	A1	20060518	WO 2005-EP12045	20051110
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM AU 2005303965 A1 20060518 AU 2005-303965 20051110 CA 2585660 A1 20060518 CA 2005-2585660 20051110 EP 1812441 A1 20070801 EP 2005-819276 20051110 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR CN 101098873 A 20080102 CN 2005-80046410 20051110 JP 2008519790 T 20080612 JP 2007-540577 20051110 BR 2005017803 A 20081021 BR 2005-17803 20051110 AR 51485 A1 20070117 AR 2005-104725 20051111 IN 2007DN03269 A 20070831 IN 2007-DN3269 20070501 US 20080096868 A1 20080424 US 2007-718730 20070507 MX 2007005644 A 20070605 MX 2007-5644 20070510 KR 2007084191 A 20070824 KR 2007-710778 20070511 GB 2004-25035 A 20041112 WO 2005-EP12045 W 20051110				
PRIORITY APPLN. INFO.:				

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
 OTHER SOURCE(S): CASREACT 144:488675; MARPAT 144:488675
 GI



- AB The invention is related to 1,4-substituted pyrazolopyrimidines I [R1 = (un)substituted Ph; R2 = (un)substituted aryl; R3 = H, (un)substituted alkyl, aryl, heterocyclyl; R4 = H, (un)substituted alkyl], and their pharmaceutically acceptable salts where one or more salt-forming groups are present, pharmaceuticals comprising them, and their use in the diagnosis and treatment or manufacture of a pharmaceutical formulation for the treatment of a disease that depends on inadequate activity of a protein kinase, especially a protein tyrosine kinase, preferably one or more of c-Abl, c-Src and/or especially Ephrin B4 receptor (EphB4) kinases; and/or one or more altered or mutated forms of any one or more of these, e.g. those forms that result in conversion of the resp. proto-oncogene into an oncogene, such as constitutively activated Bcr-Abl or v-Src. The invention is also related to the preparation of pyrazolopyrimidines I. Thus, II•TFA was prepared starting from 4-methoxyphenylhydrazine•xHCl and (ethoxymethylene)malononitrile. Pyrazolopyrimidine II•TFA inhibited EphB4 (IC₅₀ = 0.16 μmol/l).
- IT 887327-53-9P, 6-(3-Dimethylaminopropyl)-1-phenyl-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of 1,4-substituted pyrazolopyrimidines as EphB4 inhibitors)
- RN 887327-53-9 CAPLUS
- CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-[3-(dimethylamino)propyl]-1,5-dihydro-1-phenyl- (CA INDEX NAME)

10556224



OS.CITING REF COUNT: 4

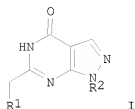
THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

REFERENCE COUNT: 4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 2004:996183 CAPLUS
 DOCUMENT NUMBER: 141:424206
 TITLE: Preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics.
 INVENTOR(S): Hendrix, Martin; Baerfacker, Lars; Erb, Christina; Hafner, Frank-Thorsten; Heckroth, Heike; Schauss, Dagmar; Tersteegen, Adrian; Van Der Staay, Franz-Josef; Van Kampen, Marja
 PATENT ASSIGNEE(S): Bayer Healthcare AG, Germany
 SOURCE: PCT Int. Appl., 96 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004099211	A1	20041118	WO 2004-EP4455	20040428
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 102004004142	A1	20041125	DE 2004-102004004142	20040128
AU 2004235915	A1	20041118	AU 2004-235915	20040428
CA 2524900	A1	20041118	CA 2004-2524900	20040428
EP 1626971	A1	20060222	EP 2004-729876	20040428
R: DE, ES, FR, GB, IT				
JP 2006525966	T	20061116	JP 2006-505294	20040428
RU 2383546	C2	20100310	RU 2005-138339	20040428
US 20070105876	A1	20070510	US 2005-556224	20051109
IN 2005DN05418	A	20070928	IN 2005-DN5418	20051124
ZA 2005009884	A	20070627	ZA 2005-9884	20051206
IN 2009DN05640	A	20100507	IN 2009-DN5640	20090831
PRIORITY APPLN. INFO.:			DE 2003-10320784	A 20030509
			DE 2003-1036183	A 20030807
			DE 2004-102004004142A	20040128
			WO 2004-EP4455	W 20040428
			IN 2005-DN5418	A3 20051124
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT				
OTHER SOURCE(S):		MARPAT 141:424206		
GI				



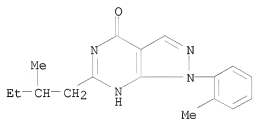
AB Title compds. [I; R1 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = (substituted) Ph, heteroaryl], were prepared Thus, reflux of 5-amino-1-(2-methylphenyl)-1H-pyrazole-4-carboxamide (preparation given) with Et cyclopentylacetate and NaH in EtOH overnight gave 30% 6-cyclopentylmethyl-1-(2-methylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one. The latter inhibited PDE9A with IC50 = 5 nM.

IT 794568-84-6P 794568-87-9P 794568-90-4P
794568-94-8P

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)

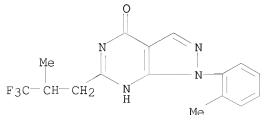
RN 794568-84-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-(2-methylbutyl)-1-(2-methylphenyl)- (CA INDEX NAME)

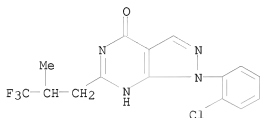


RN 794568-87-9 CAPLUS

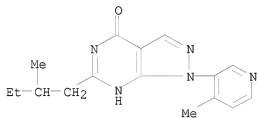
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-methylphenyl)-6-(3,3,3-trifluoro-2-methylpropyl)- (CA INDEX NAME)



RN 794568-90-4 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-chlorophenyl)-1,5-dihydro-6-(3,3,3-trifluoro-2-methylpropyl)- (CA
 INDEX NAME)



RN 794568-94-8 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1,5-dihydro-6-(2-methylbutyl)-1-(4-methyl-3-pyridinyl)- (CA INDEX NAME)

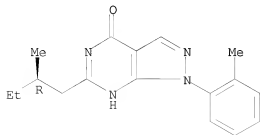


IT 794568-85-7P 794568-86-8P 794568-88-0P
 794568-89-1P 794568-91-5P 794568-92-6P
 794568-95-9P 794568-96-0P

RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN
 (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
 PREP (Preparation); USES (Uses)
 (preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors
 useful as nootropics)

RN 794568-85-7 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1,5-dihydro-6-[(2R)-2-methylbutyl]-1-(2-methylphenyl)- (CA INDEX NAME)

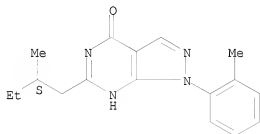
Absolute stereochemistry.



10556224

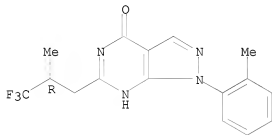
RN 794568-86-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-[(2S)-2-methylbutyl]-1-(2-methylphenyl)- (CA INDEX NAME)

Absolute stereochemistry.



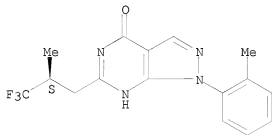
RN 794568-88-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-methylphenyl)-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]-
(CA INDEX NAME)

Absolute stereochemistry.



RN 794568-89-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-methylphenyl)-6-[(2S)-3,3,3-trifluoro-2-methylpropyl]-
(CA INDEX NAME)

Absolute stereochemistry.

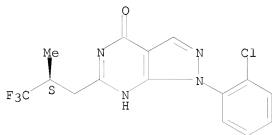


RN 794568-91-5 CAPLUS

10556224

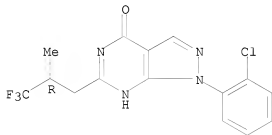
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(2-chlorophenyl)-1,5-dihydro-6-[(2S)-3,3,3-trifluoro-2-methylpropyl]-
(CA INDEX NAME)

Absolute stereochemistry.



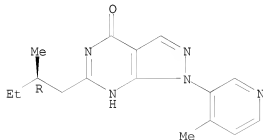
RN 794568-92-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(2-chlorophenyl)-1,5-dihydro-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]-
(CA INDEX NAME)

Absolute stereochemistry.



RN 794568-95-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-[(2R)-2-methylbutyl]-1-(4-methyl-3-pyridinyl)- (CA INDEX
NAME)

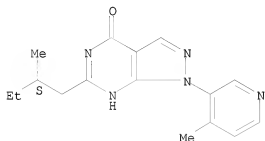
Absolute stereochemistry.



RN 794568-96-0 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-[(2S)-2-methylbutyl]-1-(4-methyl-3-pyridinyl)- (CA INDEX NAME)

Absolute stereochemistry.



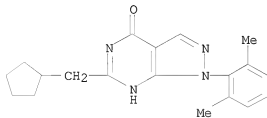
IT	794568-50-6P	794568-51-7P	794568-52-8P
	794568-53-9P	794568-54-0P	794568-55-1P
	794568-56-2P	794568-57-3P	794568-58-4P
	794568-59-5P	794568-60-8P	794568-61-9P
	794568-62-0P	794568-63-1P	794568-64-2P
	794568-65-3P	794568-66-4P	794568-67-5P
	794568-68-6P	794568-69-7P	794568-70-0P
	794568-71-1P	794568-72-2P	794568-73-3P
	794568-74-4P	794568-75-5P	794568-76-6P
	794568-77-7P	794568-78-8P	794568-79-9P
	794568-80-2P	794568-81-3P	794568-82-4P
	794568-83-5P	794568-93-7P	794568-97-1P
	794568-98-2P	794568-99-3P	794569-00-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)

RN 794568-50-6 CAPLUS

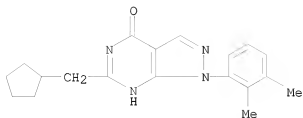
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(2,6-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)



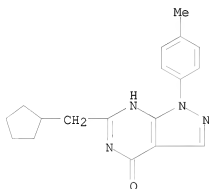
RN 794568-51-7 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(2,3-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)

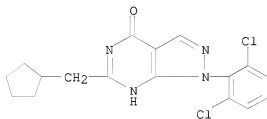
10556224



RN 794568-52-8 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(cyclopentylmethyl)-1-(4-methylphenyl)- (CA INDEX NAME)

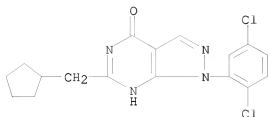


RN 794568-53-9 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(cyclopentylmethyl)-1-(2,6-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)

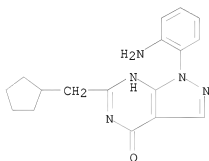


RN 794568-54-0 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(cyclopentylmethyl)-1-(2,5-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)

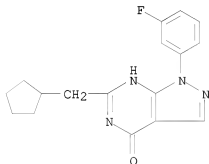
10556224



RN 794568-55-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(2-aminophenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)

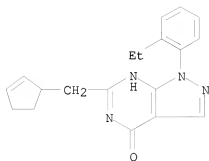


RN 794568-56-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(3-fluorophenyl)-1,5-dihydro- (CA INDEX NAME)

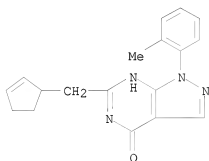


RN 794568-57-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(2-cyclopenten-1-ylmethyl)-1-(2-ethylphenyl)-1,5-dihydro- (CA INDEX NAME)

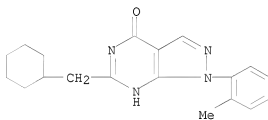
10556224



RN 794568-58-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)

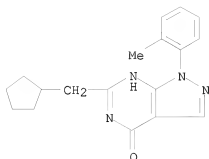


RN 794568-59-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclohexylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)

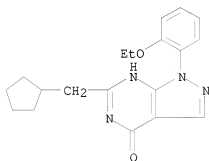


RN 794568-60-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)

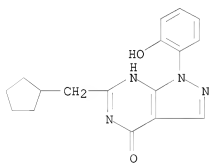
10556224



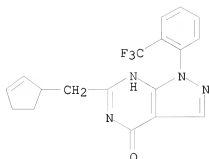
RN 794568-61-9 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(cyclopentylmethyl)-1-(2-ethoxyphenyl)-1,5-dihydro- (CA INDEX NAME)



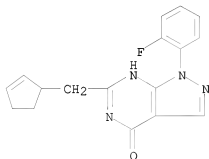
RN 794568-62-0 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-hydroxyphenyl)- (CA INDEX NAME)



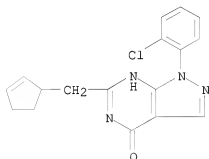
RN 794568-63-1 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-[2-(trifluoromethyl)phenyl]-
 (CA INDEX NAME)



RN 794568-64-2 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(2-cyclopenten-1-ylmethyl)-1-(2-fluorophenyl)-1,5-dihydro- (CA INDEX
 NAME)

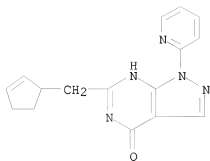


RN 794568-65-3 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-chlorophenyl)-6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro- (CA INDEX
 NAME)



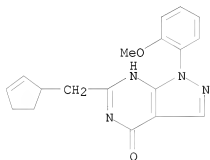
RN 794568-66-4 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-pyridinyl)- (CA INDEX NAME)

10556224



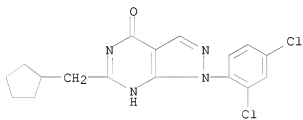
RN 794568-67-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-methoxyphenyl)- (CA INDEX NAME)



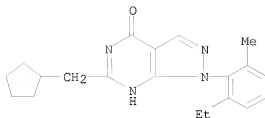
RN 794568-68-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(2,4-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)

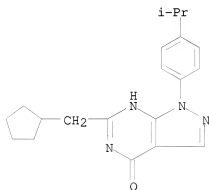


RN 794568-69-7 CAPLUS

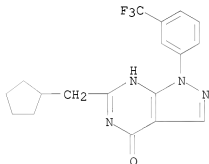
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(2-ethyl-6-methylphenyl)-1,5-dihydro- (CA INDEX NAME)



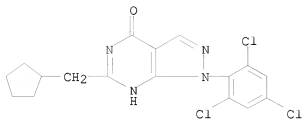
RN 794568-70-0 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(cyclopentylmethyl)-1,5-dihydro-1-[(1-methylethyl)phenyl]- (CA INDEX
 NAME)



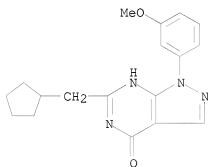
RN 794568-71-1 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(cyclopentylmethyl)-1,5-dihydro-1-[3-(trifluoromethyl)phenyl]- (CA
 INDEX NAME)



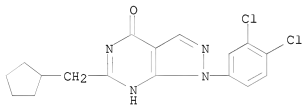
RN 794568-72-2 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(cyclopentylmethyl)-1,5-dihydro-1-(2,4,6-trichlorophenyl)- (CA INDEX
 NAME)



RN 794568-73-3 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(cyclopentylmethyl)-1,5-dihydro-1-(3-methoxyphenyl)- (CA INDEX NAME)

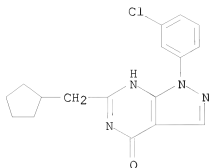


RN 794568-74-4 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(cyclopentylmethyl)-1-(3,4-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



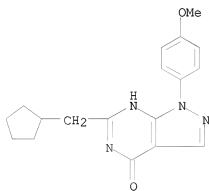
RN 794568-75-5 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(3-chlorophenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)

10556224



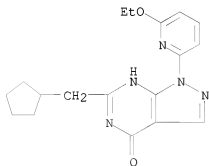
RN 794568-76-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methoxyphenyl)- (CA INDEX NAME)



RN 794568-77-7 CAPLUS

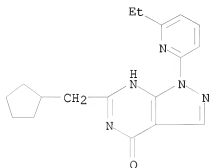
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(6-ethoxy-2-pyridinyl)-1,5-dihydro- (CA INDEX NAME)



RN 794568-78-8 CAPLUS

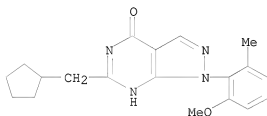
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,

6-(cyclopentylmethyl)-1-(6-ethyl-2-pyridinyl)-1,5-dihydro- (CA INDEX
NAME)



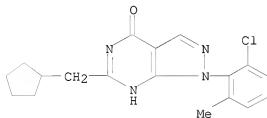
RN 794568-79-9 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(2-methoxy-6-methylphenyl)- (CA INDEX
NAME)



RN 794568-80-2 CAPLUS

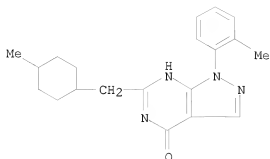
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(2-chloro-6-methylphenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX
NAME)



RN 794568-81-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-[(4-methylcyclohexyl)methyl]-1-(2-methylphenyl)- (CA INDEX
NAME)

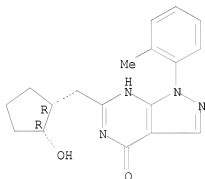
10556224



RN 794568-82-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-[[1-(2-methylphenyl)-2-hydroxycyclopentyl]methyl]-1- (2-methylphenyl)-,
rel- (CA INDEX NAME)

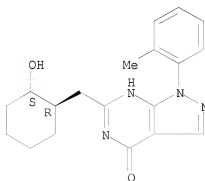
Relative stereochemistry.



RN 794568-83-5 CAPLUS

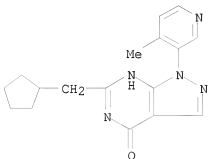
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-[[1-(2-methylphenyl)-2-hydroxycyclohexyl]methyl]-1- (2-methylphenyl)-,
rel- (CA INDEX NAME)

Relative stereochemistry.

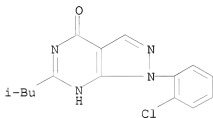


10556224

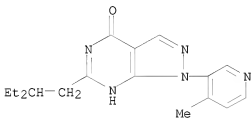
RN 794568-93-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methyl-3-pyridinyl)- (CA INDEX NAME)



RN 794568-97-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(2-chlorophenyl)-1,5-dihydro-6-(2-methylpropyl)- (CA INDEX NAME)

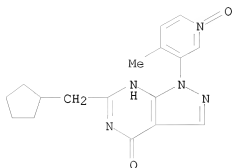


RN 794568-98-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(2-ethylbutyl)-1,5-dihydro-1-(4-methyl-3-pyridinyl)- (CA INDEX NAME)



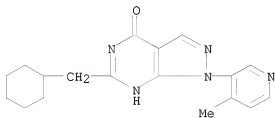
RN 794568-99-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methyl-1-oxido-3-pyridinyl)- (CA INDEX NAME)

10556224



RN 794569-00-9 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclohexylmethyl)-1,5-dihydro-1-(4-methyl-3-pyridinyl)- (CA INDEX
NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2004:996182 CAPLUS

DOCUMENT NUMBER: 141:410967

TITLE: Preparation of 6-arylmethylpyrazolopyrimidines as PDE9A inhibitors for the treatment of Alzheimer's disease

INVENTOR(S): Hendrix, Martin; Baerfacker, Lars; Erb, Christina; Hafner, Frank-Thorsten; Heckroth, Heike; Schauss, Dagmar; Tersteegen, Adrian; Van Der Staay, Franz-Josef; Van Kampen, Marja

PATENT ASSIGNEE(S): Bayer Healthcare AG, Germany

SOURCE: PCT Int. Appl., 69 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

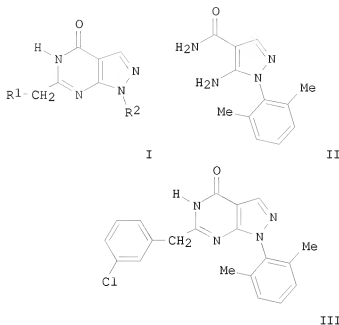
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004099210	A1	20041118	WO 2004-EP4412	20040427
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10320785	A1	20041125	DE 2003-10320785	20030509
CA 2524898	A1	20041118	CA 2004-2524898	20040427
EP 1628980	A1	20060301	EP 2004-739107	20040427
EP 1628980	B1	20100428		
R: DE, ES, FR, GB, IT				
JP 2006525963	T	20061116	JP 2006-505276	20040427
ES 2342066	T3	20100701	ES 2004-739107	20040427
US 20070161662	A1	20070712	US 2006-556437	20061010
US 7615558	B2	20091110		
US 20100035900	A1	20100211	US 2009-580725	20091016
PRIORITY APPLN. INFO.:			DE 2003-10320785	A 20030509
			WO 2004-EP4412	W 20040427
			US 2006-556437	A1 20061010

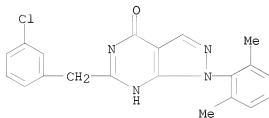
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
GI



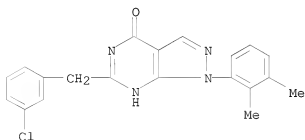
AB Title compds. I [R1 = (un)substituted Ph, pyridyl, thiophenyl, etc.; (un)substituted Ph, heteroaryl] and their pharmaceutically acceptable salts were prepared. For example, condensation-cyclization of 3-chlorophenylacetic acid Me ester and aminopyrazole II, e.g., prepared from 2,3-dimethylphenylhydrazine hydrochloride and (ethoxymethylene)propanedinitrile, afforded pyrazolopyrimidine III in 37% yield. In human guanosine cyclic 3,5'-phosphate phosphodiesterase (PDE9A) inhibition assays, 4-examples of compds. I exhibited IC50 values ranging from <30-64 nM. Compds. I are claimed useful for the treatment of Alzheimer's disease.

IT 792952-76-2P, 6-(3-Chlorobenzyl)-1-(2,6-dimethylphenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-77-3P,
6-(3-Chlorobenzyl)-1-(2,3-dimethylphenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-78-4P,
6-(3-Chlorobenzyl)-1-(4-methylphenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-79-5P, 6-(3-Chlorobenzyl)-1-(2,6-dichlorophenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-80-8P,
6-(3-Chlorobenzyl)-1-(2,5-dichlorophenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-81-9P,
1-(2-Aminophenyl)-6-(3-chlorobenzyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-82-0P, 6-(3-Chlorobenzyl)-1-(3-fluorophenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-83-1P
792952-84-2P, 6-(2-Bromobenzyl)-1-(2-methylphenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-85-3P,
6-(3-Bromobenzyl)-1-(2-methylphenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-86-4P 792952-87-5P
792952-88-6P 792952-89-7P 792952-90-0P
792952-91-1P, 6-(3-Chlorobenzyl)-1-(2-methylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-93-3P,
6-(3-Chlorobenzyl)-1-(2-ethylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-

dJpyrimidin-4-one 792952-94-4P,
 6-(3-Chlorobenzyl)-1-(2-trifluoromethylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-
 dJpyrimidin-4-one 792952-95-5P,
 6-(3-Chlorobenzyl)-1-(2-fluorophenyl)-1,5-dihydro-4H-pyrazolo[3,4-
 dJpyrimidin-4-one 792952-96-6P,
 6-(3-Chlorobenzyl)-1-(2-chlorophenyl)-1,5-dihydro-4H-pyrazolo[3,4-
 dJpyrimidin-4-one 792952-97-7P,
 6-(3-Chlorobenzyl)-1-(2-pyridinyl)-1,5-dihydro-4H-pyrazolo[3,4-dJpyrimidin-
 4-one 792952-98-8P, 6-(3-Chlorobenzyl)-1-(2-methoxyphenyl)-1,5-
 dihydro-4H-pyrazolo[3,4-dJpyrimidin-4-one
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (preparation of arylmethylpyrazolopyrimidines as PDE9A inhibitors for the
 treatment of Alzheimer's disease)
 RN 792952-76-2 CAPLUS
 CN 4H-Pyrazolo[3,4-dJpyrimidin-4-one,
 6-[(3-chlorophenyl)methyl]-1-(2,6-dimethylphenyl)-1,5-dihydro- (CA INDEX
 NAME)

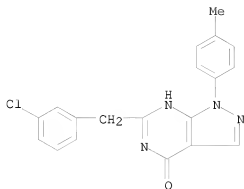


RN 792952-77-3 CAPLUS
 CN 4H-Pyrazolo[3,4-dJpyrimidin-4-one,
 6-[(3-chlorophenyl)methyl]-1-(2,3-dimethylphenyl)-1,5-dihydro- (CA INDEX
 NAME)

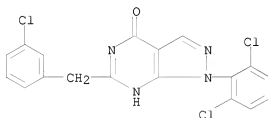


RN 792952-78-4 CAPLUS
 CN 4H-Pyrazolo[3,4-dJpyrimidin-4-one,
 6-[(3-chlorophenyl)methyl]-1-(4-methylphenyl)-1,5-dihydro- (CA INDEX
 NAME)

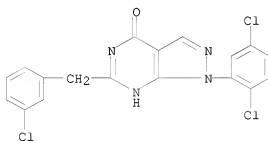
10556224



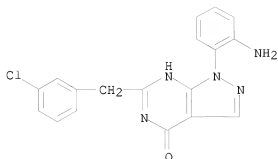
RN 792952-79-5 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-[(3-chlorophenyl)methyl]-1-(2,6-dichlorophenyl)-1,5-dihydro- (CA INDEX
 NAME)



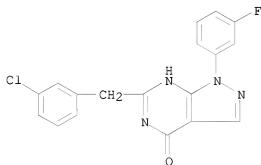
RN 792952-80-8 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-[(3-chlorophenyl)methyl]-1-(2,5-dichlorophenyl)-1,5-dihydro- (CA INDEX
 NAME)



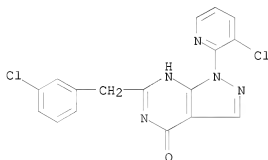
RN 792952-81-9 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-aminophenyl)-6-[(3-chlorophenyl)methyl]-1,5-dihydro- (CA INDEX NAME)



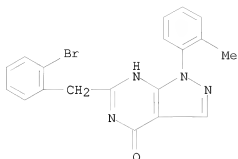
RN 792952-82-0 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-[(3-chlorophenyl)methyl]-1-(3-aminophenyl)-1,5-dihydro- (CA INDEX NAME)



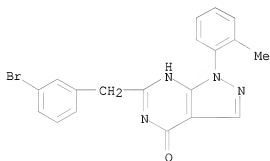
RN 792952-83-1 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-[(3-chlorophenyl)methyl]-1-(3-chloro-2-pyridinyl)-1,5-dihydro- (CA INDEX NAME)



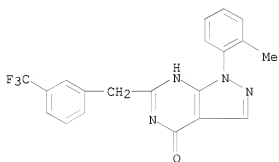
RN 792952-84-2 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-[(2-bromophenyl)methyl]-1-(2-methylphenyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



RN 792952-85-3 CAPLUS

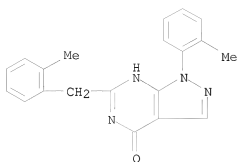
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-methylphenyl)-6-[(3-bromophenyl)methyl]- (CA INDEX NAME)

RN 792952-86-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-methylphenyl)-6-[[3-(trifluoromethyl)phenyl]methyl]- (CA
INDEX NAME)

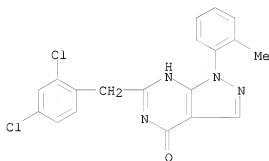
RN 792952-87-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-methylphenyl)-6-[(2-methylphenyl)methyl]- (CA INDEX
NAME)



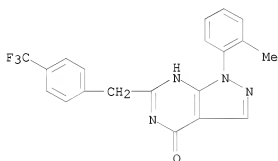
RN 792952-88-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1,5-dihydro-1-(2-methylphenyl)-6-[(2,4-dichlorophenyl)methyl]- (CA INDEX
 NAME)



RN 792952-89-7 CAPLUS

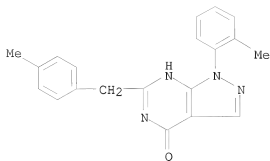
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1,5-dihydro-1-(2-methylphenyl)-6-[[4-(trifluoromethyl)phenyl]methyl]- (CA
 INDEX NAME)



RN 792952-90-0 CAPLUS

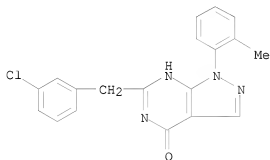
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1,5-dihydro-1-(2-methylphenyl)-6-[(4-methylphenyl)methyl]- (CA INDEX
 NAME)

10556224



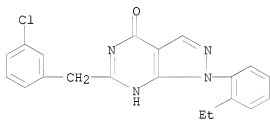
RN 792952-91-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3-chlorophenyl)methyl]-1-(2-methylphenyl)- (CA INDEX
NAME)



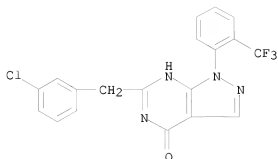
RN 792952-93-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3-chlorophenyl)methyl]-1-(2-ethylphenyl)-1,5-dihydro- (CA INDEX NAME)

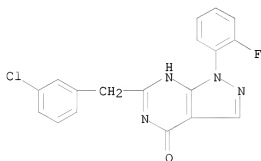


RN 792952-94-4 CAPLUS

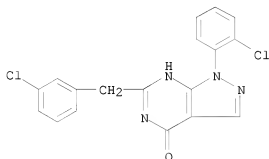
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3-chlorophenyl)methyl]-1-[2-(trifluoromethyl)phenyl]- (CA
INDEX NAME)



RN 792952-95-5 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-[(3-chlorophenyl)methyl]-1-(2-fluorophenyl)-1,5-dihydro- (CA INDEX
 NAME)

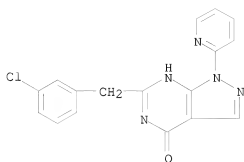


RN 792952-96-6 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(2-chlorophenyl)-6-[(3-chlorophenyl)methyl]-1,5-dihydro- (CA INDEX
 NAME)



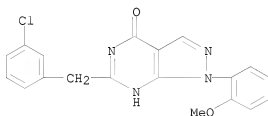
RN 792952-97-7 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-[(3-chlorophenyl)methyl]-1,5-dihydro-1-(2-pyridinyl)- (CA INDEX NAME)

10556224



RN 792952-98-8 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3-chlorophenyl)methyl]-1,5-dihydro-1-(2-methoxyphenyl)- (CA INDEX
NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:891929 CAPLUS

DOCUMENT NUMBER: 139:381500

TITLE: Preparation of pyrazolo[3,4-d]pyrimidin-4-ones as herbicides and/or nematocides

INVENTOR(S): Linker, Karl-Heinz; Andree, Roland; Hoischen, Dorothee; Schwarz, Hans-Georg; Drewes, Mark Wilhelm; Dahmen, Peter; Feucht, Dieter; Pontzen, Rolf; Loesel, Peter

PATENT ASSIGNEE(S): Bayer CropScience AG, Germany

SOURCE: Ger. Offen., 36 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

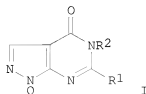
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10219435	A1	20031113	DE 2002-10219435	20020502
IN 2003MU00379	A	20050211	IN 2003-MU379	20030417
CA 2484997	A1	20031113	CA 2003-2484997	20030422
WO 2003093269	A2	20031113	WO 2003-EP4137	20030422
WO 2003093269	A3	20040408		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003224111	A1	20031117	AU 2003-224111	20030422
EP 1504005	A2	20050209	EP 2003-720510	20030422
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003009873	A	20050426	BR 2003-9873	20030422
JP 2005531549	T	20051020	JP 2004-501408	20030422
US 20050209251	A1	20050922	US 2005-512834	20050519
PRIORITY APPLN. INFO.:			DE 2002-10219435	A 20020502
			WO 2003-EP4137	W 20030422

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 139:381500

GI



AB Title compds. [I; Q = NO2, cyano, halo, (halogenated) alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, (hetero)aryl; R1 = H, (substituted) alkyl, alkoxy, carbonyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, heterocyclyl; R2 = H, (substituted) alkyl, alkenyl, alkynyl], were prepared. Thus, a mixture of 5-amino-1-(3-chloro-5-trifluoromethylpyridin-2-yl)pyrazole-4-carboxamide, CH(OMe)3, p-toluenesulfonic acid, and toluene was refluxed for 12 h followed by further addition of CH(OMe)3 and reflux for 12 h under stirring to give 44% 1-(3-chloro-5-trifluoromethylpyridin-2-yl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one. I were said to show very strong pre- and postemergent herbicidal activity, good crop tolerance, and good nematocidal activity.

IT	1053783-27-9	1053783-28-0	1053783-32-6
	1053783-35-9	1053783-56-4	1053783-57-5
	1053783-58-6	1053783-61-1	1053783-62-2
	1053783-64-4	1053783-68-8	1053783-73-5
	1053783-77-9	1053783-82-6	1053783-83-7
	1053783-90-6	1053783-93-9	1053783-95-1
	1053783-96-2	1053783-99-5	1053784-26-1

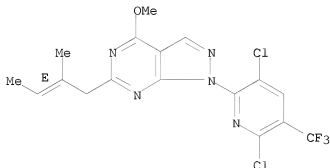
RL: PRPH (Prophetic)

(Preparation of pyrazolo[3,4-d]pyrimidin-4-ones as herbicides and/or nematocides)

RN 1053783-27-9 CAPLUS

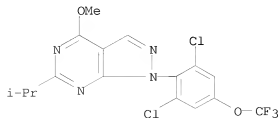
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-4-methoxy-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 1053783-28-0 CAPLUS

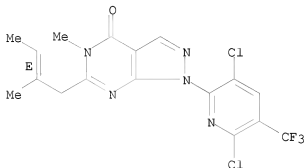
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethoxy)phenyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)



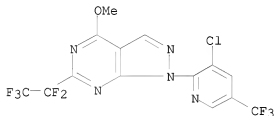
10556224

RN 1053783-32-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-
[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

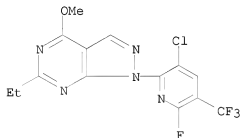
Double bond geometry as shown.



RN 1053783-35-9 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-
4-methoxy-6-(1,1,2,2,2-pentafluoroethyl)- (CA INDEX NAME)

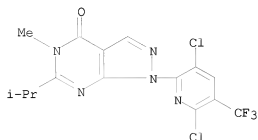


RN 1053783-56-4 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3-chloro-6-fluoro-5-(trifluoromethyl)-2-
pyridinyl]-6-ethyl-4-methoxy- (CA INDEX NAME)



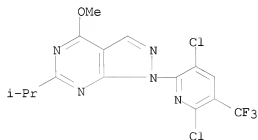
RN 1053783-57-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-(1-

methylethyl)- (CA INDEX NAME)



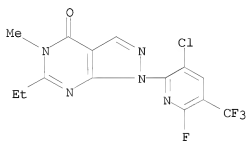
RN 1053783-58-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)



RN 1053783-61-1 CAPLUS

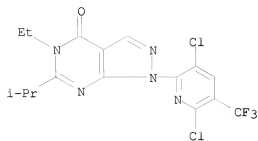
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3-chloro-6-fluoro-5-(trifluoromethyl)-2-pyridinyl]-6-ethyl-1,5-dihydro-5-methyl- (CA INDEX NAME)



RN 1053783-62-2 CAPLUS

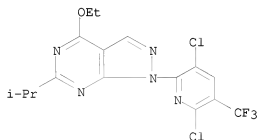
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-5-ethyl-1,5-dihydro-6-(1-methylethyl)- (CA INDEX NAME)

10556224



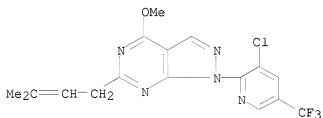
RN 1053783-64-4 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-4-ethoxy-6-(1-methylethyl)- (CA INDEX NAME)



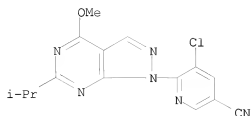
RN 1053783-68-8 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-4-methoxy-6-(3-methyl-2-buten-1-yl)- (CA INDEX NAME)



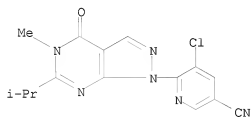
RN 1053783-73-5 CAPLUS

CN 3-Pyridinecarbonitrile, 5-chloro-6-[4-methoxy-6-(1-methylethyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]- (CA INDEX NAME)



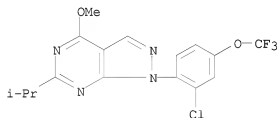
RN 1053783-77-9 CAPLUS

CN 3-Pyridinecarbonitrile, 5-chloro-6-[4,5-dihydro-5-methyl-6-(1-methylethyl)-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl]- (CA INDEX NAME)



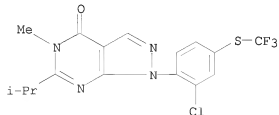
RN 1053783-82-6 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2-chloro-4-(trifluoromethoxy)phenyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)



RN 1053783-83-7 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2-chloro-4-(trifluoromethylthio)phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)

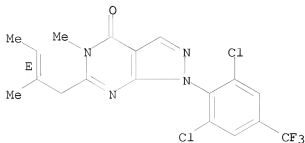


10556224

RN 1053783-90-6 CAPLUS

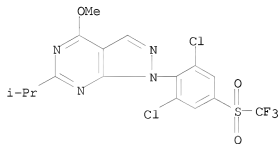
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 1053783-93-9 CAPLUS

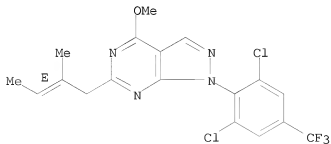
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-[(trifluoromethyl)sulfonyl]phenyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)



RN 1053783-95-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-methoxy-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

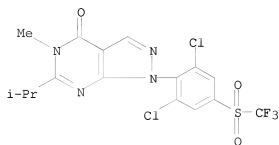
Double bond geometry as shown.



RN 1053783-96-2 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,

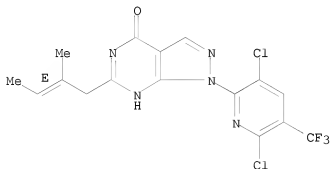
1-[2,6-dichloro-4-[(trifluoromethyl)sulfonyl]phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)



RN 1053783-99-5 CAPLUS

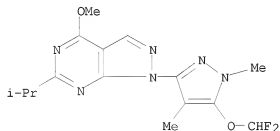
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3,6-dichloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.



RN 1053784-26-1 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[5-(difluoromethoxy)-1,4-dimethyl-1H-pyrazol-3-yl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)



IT	623584-59-8P	623584-60-1P	623584-61-2P
	623584-62-3P	623584-63-4P	623584-64-5P
	623584-65-6P	623584-66-7P	623584-67-8P
	623584-68-9P	623584-69-0P	623584-70-3P

623584-71-4P 623584-72-5P 623584-78-1P

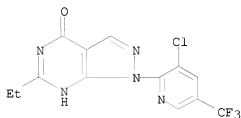
623584-98-5P 623584-99-6P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazolopyrimidinones as herbicides and/or nematocides)

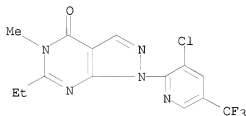
RN 623584-59-8 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-6-ethyl-1,5-dihydro- (CA
INDEX NAME)



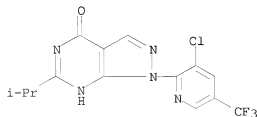
RN 623584-60-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-6-ethyl-1,5-dihydro-5-methyl-
(CA INDEX NAME)



RN 623584-61-2 CAPLUS

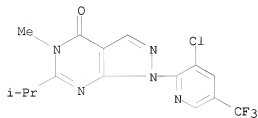
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-(1-methylethyl)-
(CA INDEX NAME)



RN 623584-62-3 CAPLUS

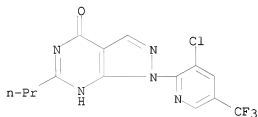
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-(1-

methylethyl)- (CA INDEX NAME)



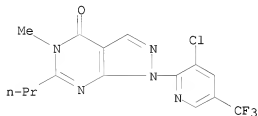
RN 623584-63-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-propyl- (CA
INDEX NAME)



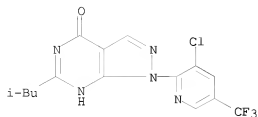
RN 623584-64-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-propyl-
(CA INDEX NAME)

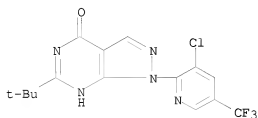


RN 623584-65-6 CAPLUS

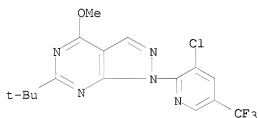
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-(2-
methylpropyl)- (CA INDEX NAME)



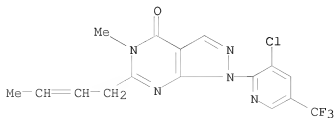
RN 623584-66-7 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-6-(1,1-dimethylethyl)-1,5-
 dihydro- (CA INDEX NAME)



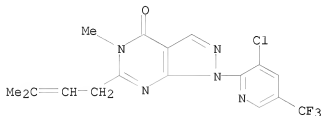
RN 623584-67-8 CAPLUS
 CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-
 6-(1,1-dimethylethyl)-4-methoxy- (CA INDEX NAME)



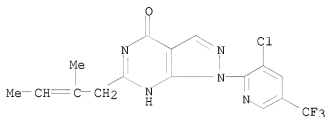
RN 623584-68-9 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-(2-buten-1-yl)-1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-
 5-methyl- (CA INDEX NAME)



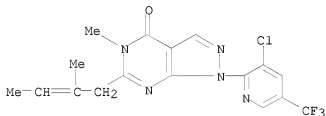
RN 623584-69-0 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-(3-methyl-2-buten-1-yl)- (CA INDEX NAME)

RN 623584-70-3 CAPLUS

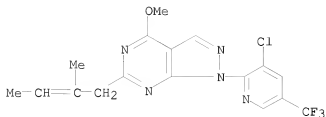
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-(2-methyl-2-buten-1-yl)- (CA INDEX NAME)

RN 623584-71-4 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-5-methyl-6-(2-methyl-2-buten-1-yl)- (CA INDEX NAME)

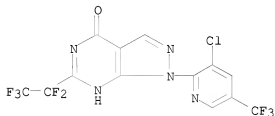
RN 623584-72-5 CAPLUS

CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-4-methoxy-6-(2-methyl-2-buten-1-yl)- (CA INDEX NAME)



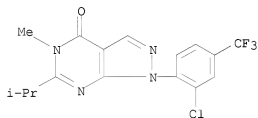
RN 623584-78-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-1,5-dihydro-6-(1,1,2,2,2-pentafluoroethyl)- (CA INDEX NAME)



RN 623584-98-5 CAPLUS

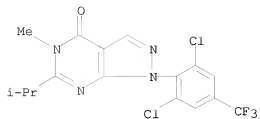
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[2-chloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)



RN 623584-99-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)

10556224



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L5 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:736859 CAPLUS

DOCUMENT NUMBER: 140:163756

TITLE: Design, synthesis, and antimicrobial activity of some new pyrazolo[3,4-d]pyrimidines

AUTHOR(S): Abdel-Gawad, Soad M.; Ghorab, M. M.; El-Sharief, A. M. Sh.; El-Telbany, F. A.; Abdel-Alla, M.

CORPORATE SOURCE: Department of Chemistry, Faculty of Science (Girl's), Al-Azhar University, Cairo, Egypt

SOURCE: Heteroatom Chemistry (2003), 14(6), 530-534

CODEN: HETCE8; ISSN: 1042-7163

PUBLISHER: John Wiley & Sons, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:163756

AB 2-Benzyl- and 2-aryloxymethyl-3-amino-1-phenyl-pyrazolo[3,4-d]pyrimidine-4-ones were synthesized by reacting arylacetyl amino derivs. with hydrazine hydrate. Thionation of the above compds. by action of P2S5 in pyridine yielded 2-aryloxy-methyl-3-amino-1-phenyl-pyrazolo[3,4-d]pyrimidin-4-thiones. 2,5-Diphenyl-2,3-dihydro-1H-pyrazolo[5',1':4:5]-pyrazolo[3,4-d]pyrimidine-8-one was also obtained via reaction of ethyl-2-cinnamoylamino-1-phenyl-pyrazole-4-carboxylate with hydrazine hydrate. The prepared compds. were screened in vitro for their antimicrobial activity. Some of the tested compds. were found to be active at 100 µg/mL compared with reference compds. (Ampicillin and Trivid) as antibacterial agents and claforan as antifungal agent.

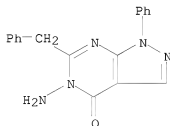
IT 654069-43-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(design, synthesis, and antibacterial activity of some new pyrazolo[3,4-d]pyrimidines from a phenylpyrazole carboxylate)

RN 654069-43-9 CAPLUS

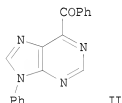
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-amino-1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)



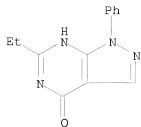
OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 1998:226504 CAPLUS
 DOCUMENT NUMBER: 128:282737
 ORIGINAL REFERENCE NO.: 128:55970h,55971a
 TITLE: Catalytic action of azolium salts. IX. Synthesis of
 6-aroysl-9H-purines and their analogs by nucleophilic
 aroylation catalyzed by imidazolium or benzimidazolium
 salt
 AUTHOR(S): Miyashita, Akira; Suzuki, Yumiko; Iwamoto, Ken-Ichi;
 Higashino, Takeo
 CORPORATE SOURCE: School of Pharmaceutical Sciences, University of
 Shizuoka, Shizuoka, 422, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1998), 46(3),
 390-399
 CODEN: CPBTAL; ISSN: 0009-2363
 PUBLISHER: Pharmaceutical Society of Japan
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 128:282737
 GI



AB In the presence of 1,3-dimethylimidazolium iodide (I),
 6-chloro-9-phenyl-9H-purine and 4-chloro-5,6-dimethylpyrrolo[2,3-
 d]pyrimidines underwent nucleophilic aroylation with arenecarbaldehydes to
 give the corresponding fused aroylpyrimidines, e.g. II.
 1,3-Dimethylbenzimidazolium iodide (III) was an effective catalyst for the
 similar synthesis of 7-aroysl-3-phenyl-3H-1,2,3-triazolo[4,5-d]pyrimidines.
 In the synthesis of 4-aroysl-1H-pyrazolo[3,4-d]pyrimidines, both azolium
 salts I and III were effective as catalysts. Moreover,
 4-aroysl-7H-pyrrolo[2,3-d]pyrimidines were obtained in good yields via the
 4-tosyl derivs., in the presence of catalytic amts. of sodium
 p-toluenesulfinate and the imidazolium salt I. This catalytic aroylation
 was found to be a facile and useful method for the synthesis of
 6-aroysl-9H-purines and their analogs.
 IT 5394-42-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis of 6-aroysl-9H-purines and analogs via nucleophilic
 aroylation catalyzed by imidazolium or benzimidazolium salt)
 RN 5394-42-3 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA
 INDEX NAME)



OS.CITING REF COUNT:	25	THERE ARE 25 CAPLUS RECORDS THAT CITE THIS RECORD (25 CITINGS)
REFERENCE COUNT:	25	THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1992:174107 CAPLUS

DOCUMENT NUMBER: 116:174107

ORIGINAL REFERENCE NO.: 116:29471a, 29474a

TITLE: Versatile synthesis of
6-alkyl(aryl)-1H-pyrazolo[3,4-d]pyrimidin-4[5H]-ones
AUTHOR(S): Reddy, K. Hemender; Reddy, A. Panduranga;
Veeranagaiah, V.

CORPORATE SOURCE: Nizam Coll., Osmania Univ., Hyderabad, 500 001, India

SOURCE: Indian Journal of Chemistry, Section B: Organic
Chemistry Including Medicinal Chemistry (1992),
31B(3), 163-6

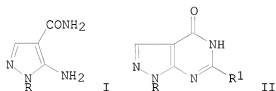
CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 116:174107

GI



AB Condensation of 5-amino-1H-pyrazole-4-carboxamide (I, R = H) with various aromatic aldehydes furnishes 6-substituted 1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones II (R1 = Ph, substituted Ph) via the intermediate 5-(N-arylideneamino)pyrazole-4-carboxamides. II were also synthesized by the reaction of I (R = H) with aromatic carboxylic acids in polyphosphoric acid (PPA) or polyphosphate ester (PPE). Similar treatment of I (R = Ph, Me) with aromatic aldehydes and aromatic carboxylic acids gives exclusively 6-substituted 1-methyl/phenyl-1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones. The title compds. have been also synthesized by the reaction of I with arylideneanilines.

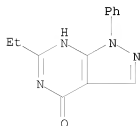
IT 5394-42-3P 130925-64-3P 139954-52-2P

139954-53-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

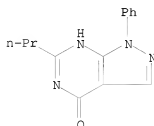
RN 5394-42-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA
INDEX NAME)

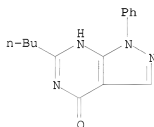


10556224

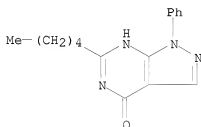
RN 130925-64-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-propyl- (CA
INDEX NAME)



RN 139954-52-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-butyl-1,5-dihydro-1-phenyl- (CA
INDEX NAME)



RN 139954-53-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-pentyl-1-phenyl- (CA
INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L5 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1991:429256 CAPLUS

DOCUMENT NUMBER: 115:29256

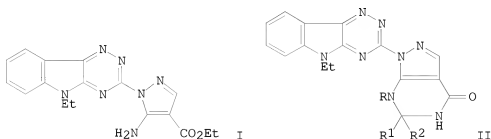
ORIGINAL REFERENCE NO.: 115:5149a,5152a

TITLE: Synthesis of ethyl-5-amino-1-(5-ethyl-5H-1,2,4-triazino[5,6-b]indol-3-yl)-1H-pyrazole-4-carboxylate and pyrazolo[3,4-d]pyrimidine derivatives
 Younes, M. I.; Abbas, H. H.; Metwally, S. A. M.
 Fac. Sci., Assiut Univ., Quena, Egypt
 Pharmazie (1991), 46(2), 98-100
 CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



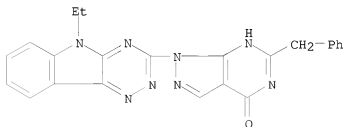
AB Ethoxymethylene cyanoacetate reacts with 5-ethyl-3-hydrazino-5H-1,2,4-triazino[5,6-b]indole to give amino(triazinoindolyl)pyrazolecarboxylate (I). I reacts with urea, thiourea and benzylnitrile to give pyrazolo[3,4-d]pyrimidine derivs. II (R = H, R₁R₂ = O, S; R₁ = bond, R₂ = CH₂Ph, resp.). The reaction of I with other reagents such as acid chlorides, acid anhydrides, hydrazines and ammonium thiocyanate was also studied.

IT 134513-78-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 134513-78-3 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 1-(5-ethyl-5H-1,2,4-triazino[5,6-b]indol-3-yl)-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)

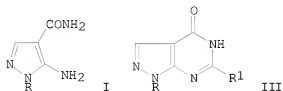


OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS

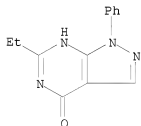
10556224

RECORD (13 CITINGS)

L5 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 1991:6429 CAPLUS
 DOCUMENT NUMBER: 114:6429
 ORIGINAL REFERENCE NO.: 114:1267a,1270a
 TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives.
 XVIII. Facile preparation of
 1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones
 Miyashita, Akira; Iijima, Chihoko; Higashino, Takeo;
 Matsuda, Hideaki
 AUTHOR(S): Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan
 CORPORATE SOURCE: Heterocycles (1990), 31(7), 1309-14
 SOURCE: CODEN: HTCYAM; ISSN: 0385-5414
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 114:6429
 GI

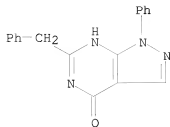


AB Reaction of 5-amino-1-phenyl-1H-pyrazole-4-carboxamide (I, R = Ph) with
 R1CO2R2 (II, R1 = H, Me, Et, Pr, Me2CH, PHCH2, CO2Et, Ph; R2 = Me, Et) in
 the presence of EtONa-EtOH gave 1-phenylpyrazolopyrimidinones III (R =
 Ph). Similar treatment of I (R = Me) with II gave III (R = Me).
 IT 5394-42-3P 94331-62-1P 130925-64-3P
 130925-65-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 5394-42-3 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA
 INDEX NAME)

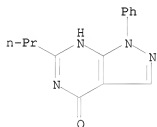


RN 94331-62-1 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)-
 (CA INDEX NAME)

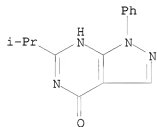
10556224



RN 130925-64-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-propyl- (CA INDEX NAME)



RN 130925-65-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(1-methylethyl)-1-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

L5 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1977:567969 CAPLUS

DOCUMENT NUMBER: 87:167969

ORIGINAL REFERENCE NO.: 87:26547a,26550a

TITLE: Synthesis of condensed heterocyclic systems of pyrazole

AUTHOR(S): Alonso, G.; Madronero, R.; Nebreda, L.

CORPORATE SOURCE: Inst. Quim. Med., Madrid, Spain

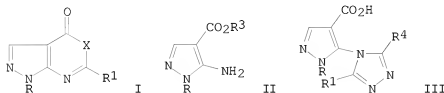
SOURCE: Anales de Química (1968-1979) (1976), 72(11-12), 897-901

CODEN: ANQUBU; ISSN: 0365-4990

DOCUMENT TYPE: Journal

LANGUAGE: Spanish

GI



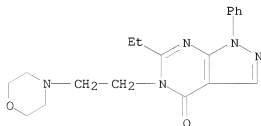
AB Pyrazolopyrimidines I (R = Ph, 2-ClC₆H₄; R₁ = Me, Et; X = NR₂, R₂ = morpholinoethyl, morpholinopropyl, NH₂, NHP) were prepared by condensing EtOCH₂C(CN)CO₂Et with RNHNH₂, hydrolyzing II (R₃ = Et), cyclizing II (R₃ = H) with (R₁CO)₂O, and treating I (X = O), with R₂NH₂. Reaction of I (X = O) with H₂NNHCO₂Et gave I (X = NNHCO₂Et), whereas R₄CONHNH₂ (R₄ = CHMe₂, CH₂CN, 2-furyl, 3-pyridyl, 1-naphthyl, 2-naphthyl, 3-indolyl, 2-indolyl, Me, Ph, PhCH₂) gave III and 1-naphthylacetylhydrazine gave a mixture of I (X = NNHCOCH₂C₁₀H₇) and III (R₄ = 1-naphthylmethyl).

IT 64257-08-5P 64257-09-6P 64257-10-9P

64257-17-6P 64257-19-8P

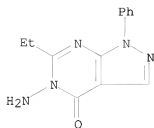
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 64257-08-5 CAPLUS

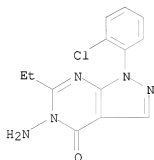
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-amino-6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)
6-ethyl-1,5-dihydro-5-[2-(4-morpholinyl)ethyl]-1-phenyl-

RN 64257-09-6 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-amino-6-ethyl-1,5-dihydro-1-phenyl-
(CA INDEX NAME)

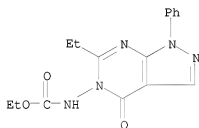


RN 64257-10-9 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-amino-1-(2-chlorophenyl)-6-ethyl-1,5-dihydro- (CA INDEX NAME)

RN 64257-17-6 CAPLUS

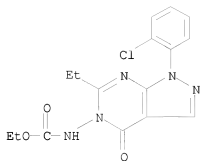
CN Carbamic acid, (6-ethyl-1,4-dihydro-4-oxo-1-phenyl-5H-pyrazolo[3,4-d]pyrimidin-5-yl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 64257-19-8 CAPLUS

CN Carbamic acid, [1-(2-chlorophenyl)-6-ethyl-1,4-dihydro-4-oxo-5H-pyrazolo[3,4-d]pyrimidin-5-yl]-, ethyl ester (9CI) (CA INDEX NAME)

10556224



OS.CITING REF COUNT: 2

THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

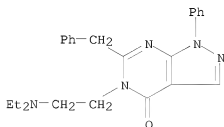
L5 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 1965:22609 CAPLUS
 DOCUMENT NUMBER: 62:22609
 ORIGINAL REFERENCE NO.: 62:4037c-e
 TITLE: Pyrazolo[3,4-d]pyrimidines
 PATENT ASSIGNEE(S): CIBA Ltd.
 SOURCE: 7 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 973361		19641028	GB 1961-17103	19610510
			CH	19600511

PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.
 AB The title compds. (I) were prepared by alkylating a 1,6-disubstituted 4-hydroxypyrazolo[3,4-d]pyrimidine with a dialkylaminoalkyl chloride or Me₂SO₄. Thus, a solution of 1.15 g. Na in 40 ml. EtOH was added to 14.1 g. 1-sec-butyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine followed by 7.5 g. Et₂NCH₂CH₂Cl and the mixture refluxed 4 hrs. to give the hydrochloride of I (R₁ = sec-Bu, R₂ = Et₂NCH₂CH₂, R₃ = PhCH₂), m. 147-8°. The following I were prepared similarly (R₁, R₂, R₃, m.p. free base, and m.p. hydrochloride given): iso-Pr, Me, PhCH₂, 96-7°, --; iso-Pr, Me₂NCH₂CH₂, PhCH₂, 115-17°, 229-31°; iso-Pr, Et₂NCH₂CH₂, PhCH₂, --, 202-3°; iso-Pr, Et₂N(CH₂)₃, PhCH₂, 70-1°, 173-5°; Me, Et₂NCH₂CH₂, PhCH₂, 83-5°, 219°; Ph, Et₂NCH₂CH₂, PhCH₂, 103-5°, 225°; iso-Pr, Et₂NCH₂CH₂, Me, --, --; iso-Pr, Me, iso-Pr, 75-7°, --; iso-Pr, Et₂NCH₂CH₂, iso-Pr, --(b₀.05 138-40°), --; iso-Pr, Et₂NCH₂CH₂, Ph₂CH, 124-5°, --. The title compds. had coronary dilating properties.

IT 1177-04-4
 (Derived from data in the 7th Collective Formula Index (1962-1966))
 RN 1177-04-4 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)-,
 hydrochloride (1:1) (CA INDEX NAME)



● HCl

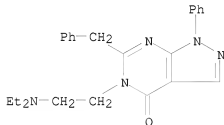
IT 1254-49-5P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-

10556224

101405-08-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-, hydrochloride
RL: PREP (Preparation of)

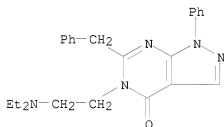
RN 1254-49-5 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA
INDEX NAME)



RN 101405-08-7 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)-,
hydrochloride (1:?) (CA INDEX NAME)



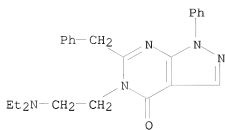
● x HCl

L5 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1965:22608 CAPLUS
 DOCUMENT NUMBER: 62:22608
 ORIGINAL REFERENCE NO.: 62:4037a-c
 TITLE: O-(α -Tetrahydropyranyl)-S-alkoxycarbonyl
 thiamines with vitamin B1 activity
 INVENTOR(S): Takamizawa, Akira; Hirai, Kentaro
 PATENT ASSIGNEE(S): Shionogi & Co., Ltd.
 SOURCE: 17 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR M2755		19640928	FR	
DE 1226586			DE	
PRIORITY APPLN. INFO.:			JP	19620727
OTHER SOURCE(S):		MARPAT 62:22608		
GI	For diagram(s), see printed CA Issue.			
AB	<p>I (R = 2-pyranyl) have a rapid and long-lasting vitamin B1 activity. They are prepared by the reaction of I (R = H, II) with 4H-dihydropyran in the presence of an acid catalyst. II are prepared from the alkali salts III (where M = Na or K) of the thiol form of thiamine (IV) with compds. XCO₂YR, where X is a halogen atom. Thus, 0.35 mL. HCl is added to a suspension of 1 g. S-ethoxycarbonylthiamine (V) in 10 mL. 4H-dihydropyran, the mixture stirred, the separated crystals are taken up in H₂O, the solution is shaken with Et₂O, and NH₄OH added to precipitate 0.80 g. O-(α-tetrahydropyranyl)-S-(ethoxycarbonyl)thiamine, m. 73-4° (H₂O + EtOH). For the preparation of V, m. 140° (decomposition) (AcOEt), IV.HCl is dissolved in aqueous NaOH, the solution saturated with NaCl, and ClCO₂Et added. Other compds. prepared are O-(α-tetrahydropyranyl)-S-(butoxycarbonyl)thiamine, m. 125°; S-butoxycarbonylthiamine, m. 139-40° (decomposition); O-(α-tetrahydropyranyl)-S-ethylthiocarbonylthiamine, m. 102-3°; and S-ethylthiocarbonylthiamine, m. 136-7° (decomposition).</p>			
IT	1177-04-4 (Derived from data in the 7th Collective Formula Index (1962-1966))			
RN	1177-04-4 CAPLUS			
CN	<p>4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)-, hydrochloride (1:1) (CA INDEX NAME)</p>			

10556224



● HCl

L5 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN
 ACCESSION NUMBER: 1963:469189 CAPLUS
 DOCUMENT NUMBER: 59:69189
 ORIGINAL REFERENCE NO.: 59:12820a-h,12821a
 TITLE: Pyrazolo[3,4-d]pyrimidines
 INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max
 PATENT ASSIGNEE(S): CIBA Ltd.
 SOURCE: 7 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1149013		19630522	DE CH	19600511

PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

AB 4-Oxo-4,5-dihydropyrazolo[3,4-d]pyrimidines (I), possessing vasodilating ability, are described in which R1 = H, alkyl or phenyl group, R2 = H or lower alkyl group, R3 = HO, halogen, NR5R6 (R5 and R6 = H, alkyl groups or joined together through O, S, or N) (or the position may be unsubstituted), R4 = alkyl or aralkyl group. The most active compds., I (R1 = iso-Pr, R2 = H, R3 = Et2NCH2CH2, R4 = PhCH2) (II) and I (R1 = sec-Bu, R2 = H, R3 = Et2NCH2CH2, R4 = PhCH2) (III) at a concentration of 10 γ /ml. increase coronary blood flow 78-73% in the Langendorf isolated dog heart procedure. In the same test, 1-isopropyl-4-diethylaminopyrazolo-[3,4-d]pyrimidine (CA 55, 13457a) at the same concentration causes an increase of 60%. In the compds. described

below

R2 = H. Na (2.3 g.) is finely dispersed in 50 ml. PhCH2CN and 9.9 g. 2-isopropyl-3-amino-4-carbethoxypyrazole (IV) added. The mixture is heated to 110-20° with stirring for 4 hrs. and cooled, 100 ml. alc. is added, and the mixture evaporated to dryness in vacuo. The residue is taken into 150 ml. 2N NaOH, extracted with CHCl3 to remove undissolved material and adjusted to pH 5 to 6 with 6N HCl to yield 1-isopropyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (V), m. 165-6° (alc.). V in 30 ml. N NaOH treated with Me2SO4 gave I (R1 = iso-Pr, R3 = Me, R4 = PhCH2) (VI), m. 96-7°. The procedure similar to that used for the preparation of IV is used to prepare 1-sec-butyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (VII), m. 154-5°. A solution of 1.15 g. Na in 40 ml. absolute alc. is added to 14.4 g. VII in 60 ml. absolute alc. and refluxed 4 hrs. after the addition of 7.5 g. Et2NCH2CH2Cl to give after HCl treatment 15.4 g. III.HCl, m. 147-8°. Similarly, 13.4 g. V is allowed to react with 1.2 g. Na in 300 ml. absolute EtOH, then with 5.5 g. Me2NCH2CH2Cl to yield 10.2 g. I (R1 = iso-Pr, R3 = Me2NCH2CH2, R4 = PhCH2) (VIII), m. 115-17°; VIII.HCl m. 229-31°. V, as the Na salt, is allowed to react with Et2NCH2CH2Cl to yield I (R1 = iso-Pr, R3 = Et2NCH2CH2, R4 = PhCH2).HCl, m. 202-3°. When V, as the Na salt, is allowed to react with Et2NCH2CH2CHCl, II.HCl, m. 173-5°, is isolated. 1-Methyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (IX) is prepared from 2-methyl-3-amino-4-carbethoxypyrazole and PhCH2CN (X) by the procedure for the preparation of V. The reaction of 12 g. IX with 1.2 g. Na in 25 ml. absolute alc. followed by the addition of 6 g. Et2NCH2CH2Cl leads to the isolation of I (R1 = Me, R3 = Et2NCH2CH2, R4 = PhCH2) (XI), m. 83-5° XI.HCl m.

219°. Likewise, 2-phenyl-3-amino-4-carbethoxypyrazole and X yields 1-phenyl-6-benzyl-4-hydroxypyrazolo[3,4-d]pyrimidine, m. 264-5° which is allowed to react as the Na salt with Et2 NCH2CH2Cl to give I (R1 = Ph, R3 = Et2NCH2CH2, R4 = PhCH2) (XII), m. 103 5° XII.HCl m. 225°. To an ice-cooled solution of 9.9 g. IV in 50 ml. MeCN is added 2.3 g. Na and the temperature of reaction kept below 30°. After the addition, the mixture is heated to 90-95° for 4 hrs., cooled, and 100 ml. EtOH added. The mixture is evaporated to dryness and residue treated with 150 ml. 2N NaOH, extracted with CHCl3 and the aqueous layer adjusted to pH 3 to 4 with 5N HCl and the precipitate crystallized from alc. to give 1-isopropyl-4-hydroxy-6-methylpyrazolo[3,4-d]pyrimidine (XIII), m. 195-6°. The reaction of 9.1 g. XII with 1.2 g. Na in 150 ml. absolute alc., followed by the addition of 7 g. Et2NCH2CH2Cl, and 4 hrs. reflux yields 7 g. I (R1 = iso-Pr, R3 = Et2NCH2CH2, R4 = Me), m. 166-8°. 1,6-Diisopropyl-4-hydroxypyrazolo[3,4-d]pyrimidine (XIV), m. 175-7°, is prepared from iso-BuCN and IV in the presence of Na. A solution of 11 g. XIV in 75 ml. 2N NaOH solution is stirred at room temperature with 6.3 g. Me2SO4 and allowed to stand overnight to yield 9 g. I (R1 = R4 = iso-Pr, R3 = Me), m. 175-7°. XIV (10 g.) is added to a solution of 1.05 g. Na in 150 ml. absolute alc., stirred 1 hr. at room temperature and 6.5 g. Et2. NCH2CH2Cl is added. The mixture is refluxed 4 hrs., evaporated to dryness in vacuo and the residue dissolved in 100 ml. N HCl, adjusted to a pH with NaOH solution and the oil that results is extracted with Et2O. The residue, after removal of the Et2O, is distilled to yield 9 g. I (R1 = R4 = iso-Pr, R3 = Et2NCH2CH2), b0.05 138-40°. A mixture of 20 g. X and 19.7 g. IV is warmed to 70° and 2.3 g. of Na in small pieces added. The mixture is heated 4 hrs. at 110-20°, allowed to cool, and the excess Na destroyed by the addition of alc. The mixture is evaporated to dryness in vacuo, the residue treated with 300 ml. H2O and 2N HCl added to adjust the pH to 3. The precipitate is removed by filtration and crystallized from petr. ether to yield 1-isopropyl-4-hydroxy-6-diphenylmethylpyrazolo[3,4-d]pyrimidine (XV), m. 226 7°. XV(5.2 g.) is added to a solution of 0.35g. Na in 150 ml. EtOH, the mixture stirred at room temperature and 2.1 g. Et2NCH2CH2Cl is added. The mixture is refluxed 4 hrs. and evaporated to dryness in vacuo and the residue crystallized from petr. ether to yield 3.8 g. I (R1 = iso-Pr, R3 = Et2NCH2CH2, R4 = PhCH2), m. 124-5°.

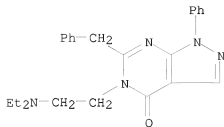
IT 1254-49-5P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-94331-62-1P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-phenyl-101405-08-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-, hydrochloride

RL: PREP (Preparation)
(preparation of)

RN 1254-49-5 CAPLUS

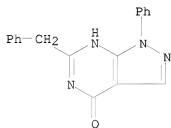
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)

10556224



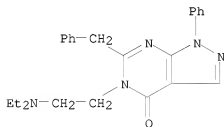
RN 94331-62-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)-
(CA INDEX NAME)



RN 101405-08-7 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)-,
hydrochloride (1:?) (CA INDEX NAME)



●x HCl

OS.CITING REF COUNT: 1

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L5 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1963:408986 CAPLUS

DOCUMENT NUMBER: 59:8986

ORIGINAL REFERENCE NO.: 59:1635g-h

TITLE: New synthesis of pyrazolo[3,4-d]pyrimidines with
dilatory effect on coronary vesselsAUTHOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max;
Burckhardt, Christoph A.

CORPORATE SOURCE: CIBA S. A., Basel, Switz.

SOURCE: Annali di Chimica (Rome, Italy) (1963), 53, 61-9

CODEN: ANCRAI; ISSN: 0003-4592

DOCUMENT TYPE: Journal

LANGUAGE: French

AB cf. *Helv. Chim. Acta* 45, 1620(1962). The position of the functional groups of 3-amino-4-carbethoxypyrazoles suggested the formation of bicyclic compds. by the action of appropriate reagents. Treatment with suitable nitriles led to a new synthesis of pyrazolo[3,4-d]pyrimidines substituted in the 6-positions, and to 6-aminopyrazolo[3,4-b]pyridines. The reaction was extended to numerous examples and the constitution of the products proved by independent syntheses (exptl. details, loc. cit.). Degradation in acid media converted the 6-substituted pyrazolopyrimidines to pyrazole derivs. Several of the compds. possessed a marked dilatory effect on the coronary vessels.

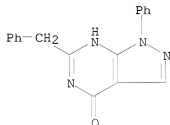
IT 94331-62-1P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,

6-benzyl-1,5-dihydro-1-phenyl-

RL: PREP (Preparation)

(preparation of)

RN 94331-62-1 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)-
(CA INDEX NAME)

L5 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1962:483251 CAPLUS

DOCUMENT NUMBER: 57:83251

ORIGINAL REFERENCE NO.: 57:16611d-i,16612a-e

TITLE: Chemotherapeutic studies in the heterocyclic series.

XXXIV. Pyrazolopyrimidines. 5. A new synthesis of pyrazolo[3,4-d]pyrimidine with coronary dilating properties

AUTHOR(S): Schmidt, P.; Eichenberger, K.; Wilhelm, M.

CORPORATE SOURCE: Ciba, Basel, Switz.

SOURCE: Helvetica Chimica Acta (1962), 45, 1620-7

CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 57:83251

AB cf. CA 53, 20070d. The condensation of 3-amino-4-carbomethoxypyrazoles with nitriles led to a new synthesis of 6-(C-substituted) pyrazolo[3,4-d]pyrimidines (I) and 6-aminopyrazolo[3,4-b]pyridines. The I could be cleaved with H₃PO₄ to 3-aminopyrazole-4-carboxamide derivs. Many of the new I caused an increase of coronary flow.

2-Isopropyl-3-amino-4-carbomethoxypyrazole (II) (19.7 g.) in 250 cc. 2N NaOH refluxed 2 hrs., cooled, treated with C, and acidified with concentrated HCl to pH 3-4 gave 14.5 g. 4-CO₂H analog (III) of II, m. 151-2° (decomposition). III (84.5 g.) in 375 cc. dioxane and 40 cc. C₅H₅N treated dropwise with stirring at 10-15° with 77.3 g. PhCH₂COCl in 125 cc. dry dioxane, stirred 1 hr. at 10° and 2 hrs. at room temperature, diluted with H₂O and aqueous HCl, and extracted with Et₂O gave 53 g. 2-isopropyl-3-phenylacetylamino-4-carboxypyrazole (IV), m. 162-3°. IV (8.61 g.) and 30 cc. Ac₂O stirred 3 hrs. at 100-10° and evaporated yielded 3.1 g. 1-isopropyl-4-oxo-6-benzylpyrazolo[3,4-d]oxazine (V), m. 162-3° (Me₂CO-petr. ether). III (30 g.) in 180 cc. dry dioxane and 16 cc. C₅H₅N treated dropwise with stirring at 10-15° with 31 g. PhCH₂COCl in 50 cc. dioxane and processed in the usual manner gave 21 g. 4-CN analog (VI) of IV, m. 140-2° (EtOH). PhCH₂CN (26.3 g.) in 250 cc. CHCl₃ and 13 cc. absolute EtOH saturated with dry HCl, kept overnight, evaporated

below 30°, the residue dissolved in 200 cc. CHCl₃, treated with 16.9 g. 2-isopropyl-3-amino-4-carbamoylpyrazole (VII) in 1800 cc. CHCl₃, refluxed 10 hrs. with stirring, filtered, and evaporated yielded 2-isopropyl-3-(1-ethoxy-2-phenylethylidenimino)-pyrazole-4-carboxamide (VIII), m. 111-14° (Et₂O). II (70 g.) and 140 g. PhCH₂CN added during 1 hr. with stirring at 90-5° to 16.5 g. powdered Na in 300 cc. dry MePh, refluxed 7 hrs. with stirring, diluted with 240 cc. absolute EtOH, evaporated, the residue dissolved in 1.2 l. N NaOH, washed with MePh, and acidified with 5N HCl to pH 5-6 gave 62.4 g. 1-isopropyl-4-oxo-6-benzyl-4,5-dihydropyrazolo [3,4-d]pyrimidine (IX), m. 164-6° (absolute EtOH); the alc. mother liquor concentrated, filtered, the residue (8.1 g.) shaken 0.5 hr. with 81 cc. CH₂Cl₂, and filtered left 4.77 g. 2-isopropyl-4-hydroxy-5-phenyl-6-aminopyrazolo[3,4-b]pyridine (X), m. 256-7° (EtOH); the CH₂Cl₂ filtrate evaporated gave 1.9 g. IX.

Similarly were prepared the following

1,6-disubstituted-4-oxo-4,5-dihydropyrazolo[3,4-d]pyrimidines (1- and 6-substituent and m.p. given): Me, PhCH₂, 233-7°; Me, p-ClC₆H₄CH₂, 268-70°; Me, 3,4,5-(MeO)3C₆H₂CH₂, 245-6°; HOCH₂CH₂, PhCH₂, 194-5°; iso-Pr, Me, 180-2°; iso-Pr, Ph, 256-8°; iso-Pr, PhCH₂, 165-6°; iso-Pr, p-ETOC₆H₄CH₂, 175-6°; cyclopentyl, PhCH₂, 189-90°; cyclohexyl, PhCH₂, 207-8°; Ph,

PhCH₂ (XIII), 263-5°. V (5.4 g.), 50 cc. C₆H₆, and 15 cc. liquid NH₃ in a sealed tube heated 8 hrs. at 100-10°, treated with 2N NaOH, and the aqueous phase acidified with 6N HCl to pH 6 gave 0.7 g. IX. VI (6.7g.) and 27.2 cc. 10% aqueous KOH in 102 cc. 3% H₂O₂ heated 10 hrs. at 70°, filtered, and acidified with 2N HCl to pH 5 yielded 6.12 g. IX, m. 163-5°. Crude VIII from 26.3 g. PhCH₂CN and 16.9 g. VII added to 18 g. Na in 315 cc. MeOH, kept overnight, refluxed 0.5 hr., filtered, evaporated, the residue shaken with 200 cc. H₂O and 200 cc. CHCl₃, and the aqueous phase acidified with 5N HCl gave 16.6 g. IX. VII (8.4 g.) and 27 g. PhCH₂CONH₂ heated 4 hrs. at 200-10°, cooled, powdered, extracted with 2N NaOH, and the alkaline extract acidified with 2N HCl to pH 3 yielded

3.2

g. IX, m. 165-6° (EtOH). II (39.4 g.) in 150 cc. dry dioxane and 16 cc. C₅H₅N treated with stirring at 10-15° during 15 min. with 31 g. PhCH₂COCl in 50 cc. dioxane, stirred 1 hr. at 10° and 2 hrs. at room temperature, treated with 130 cc. 2N HCl and 380 cc. H₂O, and extracted

with

about 1000 cc. Et₂O yielded 33 g. 2-isopropyl-3-phenylacetyl-amino-4-carbethoxypyrazole (XIV), b_{0.08} 170-5°. NaNO₂ (7 g.) and 26.8 g. X added successively with stirring at 0-5° to 268 cc. concentrated H₂SO₄, stirred 3 hrs. at 0-5°, cooled, poured onto ice, heated with stirring to 80°, cooled, filtered, the residue (about 20 g.) treated with 400 cc. saturated aqueous NaHCO₃ and 400 cc. H₂O, filtered, and

the

filtrate acidified with 2N HCl to pH 3-4 yielded 16.8 g. 1-isopropyl-4-hydroxy-5-phenyl-6-oxo-4,5-dihydropyrazolo[3,4-b]pyridine (XV), m. 322-4° (EtOH). XIV (10 g.) and 2 g. Na in 150 cc. MePh refluxed 5 hrs. with stirring, cooled to room temperature, treated with EtOH, evaporated, the residue dissolved in H₂O, washed with Et₂O, and acidified with 2N HCl gave 2.3 g. XV, m. 322-4° (aqueous EtOH). XIII (15 g.) and 100 cc. POCl₃ refluxed 6 hrs., evaporated, the residue dissolved in CHCl₃, and worked up gave 7.2 g. 1-phenyl-4-chloro-6-benzylpyrazolo[3,4-d]pyrimidine (XVI), m. 90-1° (CHCl₃-petr. ether). XVI (7 g.) and 25 g. Me₂NH in 50 cc. EtOH heated 7 hrs. at 100° in an autoclave gave 4.3 g. 4-Me₂N analog of XVI, m. 121-2° (EtOH). IX (13.4 g.) and 1.15 g. Na in 300 cc. EtOH stirred 1 hr. at room temperature, treated with 5.5 g. Me₂NCH₂CH₂Cl, refluxed 4 hrs., evaporated, the residue dissolved in 100 cc. N HCl, washed with Et₂O, basified to pH 10 with aqueous NaOH, and extracted with Et₂O yielded 13 g. 5-Me₂NCH₂CH₂ derivative (XVII) of IX, m. 115-17° (petr. ether). XVII (10 g.) and 35 cc. 85% H₃PO₄ stirred 6 hrs. at 100°, poured onto 300 g. ice, adjusted with aqueous NaOH to pH 10, filtered, and extracted with CHCl₃ gave 6 g. 2-isopropyl-3-aminopyrazole-4-carboxylic acid 2-dimethylaminoethylamide, m. 131-2° (iso-Pr₂O).

IT

94331-62-1P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1,5-dihydro-1-phenyl-
RL: PREP (Preparation)

(preparation of)

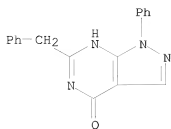
RN

94331-62-1 CAPLUS

CN

4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)-
(CA INDEX NAME)

10556224



OS.CITING REF COUNT: 1

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L5 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1958:88115 CAPLUS

DOCUMENT NUMBER: 52:88115

ORIGINAL REFERENCE NO.: 52:15540i,15541a-i,15542a-i,15543a-i

TITLE: Potential purine antagonists. VII. Synthesis of 6-alkylpyrazolo[3,4-d]pyrimidines

AUTHOR(S): Cheng, C. C.; Robins, Roland K.

CORPORATE SOURCE: New Mexico Highlands Univ., Las Vegas

SOURCE: Journal of Organic Chemistry (1958), 23, 191-200

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB Cf. C.A. 52, 13741h. A synthesis of 6-alkyl-4-hydroxypyrazolo [3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:COH (I) was devised from the corresponding 5-acylamino-4-cyanopyrazoles, R3CONHC:C(CN).CR2:N.NR1 (II) which were in turn prepared from 5-amino-4-cyanopyrazoles, R1N.N:CH.C(CN):CNH2 (III). Evidence was presented to show that the 5-acylamino-4-cyanopyrazole-4-carboxamide is an intermediate in this cyclization. Chlorination of I yielded the corresponding 6-alkyl-4-chloropyrazolo [3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:CCl (IV). Nucleophilic displacement of the Cl in IV resulted in the preparation of a large number of 6-alkylpyrazolo[3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:CNR4R5 (V). III (R1 = 3-Me) (80 g.) and 250 ml. Ac2O refluxed 10 hrs., excess Ac2O distilled in vacuo, the sirupy substance poured into 30 ml. C6H6, stirred several min., and crystallized gave 89 g. II (R1 = R2 = H, R3 = Me), crystals from H2O. Similarly II (R1 = R3 = Me, R2 = H) was prepared and the product recrystd. from H2O to a white powder. III (R1 = Ph) (150 g.) treated 19 hrs. under reflux with 200 ml. Ac2O, excess solvent removed, the residue treated with a small amount of C6H6, and Skellysolve (b. 60°), and the product isolated gave 171 g. II (R1 = Ph, R2 = H, R3 = Me) crystallized from H2O. The following II were thus prepared (R1, R2, R3, m.p., % yield, and recrystn. solvent given): H, H, Me, 221-2°, 76, H2O; Me, H, Me, 210-11°, 72, H2O; Ph, H, Me, 155-6°, 92, H2O; o-ClC6H4, H, Me, 175-5.5°, 82, alc., H2O; p-ClC6H4, H, Me, 173-5°, 96, alc, H2O; p-BrC6H4, H, Me, 175-5° (sic), 98, alc., H2O; p-ONC6H4, H, Me, 198-200°, 95, alc., H2O; p-MeC6H4, H, Me, 128°, 96, alc., H2O; AcOCH2CH2, H, Me, 155-7°, 81, alc. II (R1 = Ph, R2 = H, R3 = Me) (30 g.) added at 15-20° to 120 ml. concentrated H2SO4, the clear solution stirred 0.5 hr., then poured onto 1 kg.

ice, neutralized with concentrated NH4OH, the solid collected, washed, dried, and recrystd. from C6H6 and MeOH gave 20 g.

5-amino-1-phenylpyrazole-4-carboxamide (VI), m. 172-5°, identical

with the product obtained from the hydrolysis of

5-amino-4-cyano-1-phenylpyrazole. VI (20 g.) and 200 ml. Ac2O refluxed 15

hrs., and purification gave 15 g. 6-methyl-4-oxo-1-phenylpyrazolo

[3,4-d]-5,7-oxazine (VII), m. 184.5-5.5° (sublimed at 145°)

(C6H6-C7H16). VII (2.5 g.) kept 2 hrs. at room temperature with 200 ml. H2O

and 2 g. KOH, heated 10 hrs., acidified, and the precipitate collected gave 2 g. 5-acetamido-1-phenylpyrazole-4-carboxylic acid (VIII), m. 201-2°

(AcOH), readily lost CO2 on heating. The 5-acetylamido group was retained

in warm alkaline solution but hydrolyzed readily in cold acidic medium. VII (2 g.) left 0.5 hr. at room temperature with 100 ml. alc. NH3, heated briefly

until a solid product precipitated, and the product collected gave

5-acetamido-1-phenylpyrazole-4-carboxamide (IX), m. 301-2°, relatively unstable. The m.p. of IX was the same as that for I (R1 = Ph, R2 = Me) and was undepressed in mixed m.p. The ultraviolet absorptions for IX at 230 mμ and for I at 233 and 269 mμ, were different. Thus IX cyclized at elevated temps. during the m.p. determination I were prepared by the following method. II (R1 = R2 = H, R3 = Me) (1.5 g.); 7 ml. 10% KOH, and 15 ml. 3% H2O2 warmed 0.5 hr. at 70-5°, the mixture acidified, the solid collected, and reprecipitated with dilute KOH and AcOH gave 1.1 g. I (R1 = H, R2 = Me). II (R1 = R3 = Me, R2 = H) (121 g.) warmed 10 hrs. at 70° with 1500 ml. 3% H2O2 and 400 ml. 10% KOH gave 103 g. I (R1 = R2 = Me), needles, sublimed at 180°. II (R1 = Ph, R2 = H, R3 = Me) (14.5 g.) in 5 g. KOH and 200 ml. 3% H2O2 warmed 5 hrs. at 70-5° and acidified gave 14 g. crude I (R1 = Ph, R2 = Me), m. 298-300°. IX (1 g.) heated 20 min. at 70° with 100 ml. 10% KOH, then acidified, the solid collected and recrystd. gave 0.8 g. product identical with that from the preceding experiment I (R1 = R2 = Me) (25 g.) and 400 ml. POC13 refluxed 2 hrs., excess solvent removed, the sirup poured onto 1 kg. ice, the suspension left 15 min., extracted with CHCl3, dried, solvent removed at room temperature, and the solid isolated gave 24 g. IV (R1 = R2 = Me) as needles. I (R1 = H, R2 = Me) (50 g.) refluxed 2 hrs. with 140 ml. PhNMe2 and 1 l. POC13, excess POC13 removed, the residue poured on ice, and extracted with Et2O gave 35 g. IV (R1 = H, R2 = Me), unstable. I (R1 = p-O2NC6H4, R2 = Me) (20 g.) refluxed 3 hrs. with 250 ml. POC13 gave 17.5 g. IV (R1 = p-O2NC6H4, R2 = Me) as a yellow powder. Preparation of 1-alkyl(aryl)-6-alkyl-4-mercaptopyrazolo[3,4-d]pyrimidines X (R1 = 1-substituent, R2 = 6-substituent) was achieved by the following two methods: (method 1) I (R1 = Ph, R2 = Me) (11 g.) and 50 g. P2S6 added portionwise during 45 min. to 400 ml. Tetralin (preheated to 165°), the temperature allowed to rise to 185°, then heated 6 hrs. to 190-5°, the solution cooled overnight, filtered, the product dissolved in dilute KOH and precipitated with AcOH gave 5.5 g. X (R1 = Ph, R2 = Me); method 2) IV (R1 = Ph, R2 = Me) (14 g.) and 14 g. CS(CH2)2 in 120 ml. alc. refluxed 4 hrs., the product collected and washed well with alc. and H2O, and the product purified by precipitation from a hot basic solution with AcOH gave 11.5 g. X (R1 = Ph, R2 = Me). All the other X were prepared by essentially the same procedure as method 2. 1-Alkyl(aryl)-6-alkyl-4-alkylthiopyrazolo[3,4-d]pyrimidines (XI) (R1 = 1-substituent, R2 = 6-substituent, R3 = S-substituent) were prepared as follows: X (R1 = R2 = Me) (13 g.), 40 ml. 4N KOH, 18 g. MeI, and 30 ml. MeOH shaken 0.5 hr. in a separatory funnel, the contents left overnight at 40°, and the solid collected gave 12.5 g. XI (R1 = R2 = R3 = Me). X (R1 = Ph, R2 = Me) (1 g.) added to 200 ml. H2O containing 15 g. KOH and 21 g. EtI, treated with 100 ml. alc., refluxed 5 hrs., and reduced in volume, until an oily product solidified gave 3 g. XI (R1 = Ph, R2 = Me, R3 = Et). 4-Alkoxy-1-alkyl(aryl)-6-methylpyrazolo[3,4-d]pyrimidines (XII) (R1 = 1-substituent, R2 = O-substituent) were prepared as follows: IV (R1 = p-MeC6H4, R2 = Me) (5.5 g.) and 100 ml. alc. left 2 hrs. at room temperature with 2 g. Na in 70 ml. alc., heated 40 min. on the steam bath, and NaCl removed, the filtrate treated with 50 ml. H2O, and left overnight in the cold gave 3.1 g. XII (R1 = p-MeC6H4, R2 = Et). Other XII were prepared as above. The following N:CR2.N:CR3.C:CR1.N:CH were prepared by the above methods (R1, R2, R3, m.p., % yield, and recrystn. solvent given): H, Me, OH, 336-8°, 73.5, AcOH; H, Me, Cl, 140° (decomposition), 70.0, C6H6; H, Me, SH, above 300°, 80, reprecipitated; H, Et, OH, above

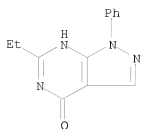
300°, 82, alc., H₂O; Me, Me, OH, 277-8°, 72.5, alc., H₂O; Me, Me, Cl, 74°, 70.2, C₇H₁₆; Me, Me, OMe, 107.5-8.5°, 67.5, MeOH; Me, Me, SH, 264-5°, 98, repptd.; Me, Me, SMe, 74-5°, 90.2, MeOH, H₂O; CH₂CH₂OH, Me, OH, 265-6°, 54.8, H₂O; Ph, Me, Cl, 85-6°, 83.5, C₇H₁₆; Ph, Me, SH, 268.5°, 83.3, repptd.; Ph, Me, OMe, 121.5-2.0°, -, MeOH; Ph, Me, OEt, 95-5.5°, -, alc.; Ph, Me, SMe, 135-7°, -, MeOH, H₂O; Ph, Me, SET, 86-8°, -, alc., H₂O; Ph, Et, OH, 295°, 88.5, alc., H₂O; Ph, Et, SH, 248-9°, 91.6, repptd.; p-MeC₆H₄, Me, OH, 298-300°, 93.6, alc., H₂O; p-MeC₆H₄, Me, Cl, 89-91°, 78.1, C₇H₁₆; p-MeC₆H₄, Me, OMe, 121-2°, 81.2, MeOH; p-MeC₆H₄, Me, OEt, 93-4°, 53, alc.; o-ClC₆H₄, Me, Cl, 121°, 77.8, C₆H₁₄; p-BrC₆H₄, Me, OH, above 315°, 86.6, alc., H₂O; p-BrC₆H₄, Me, Cl, 130.5-31°, 88.7, C₆H₁₄; p-ClC₆H₄, Me, OH, above 310°, 94.5, alc., H₂O; p-ClC₆H₄, Me, Cl, 129°, 82.6, C₇H₁₆; p-ClC₆H₄, Me, SH, above 305°, 75.2, repptd.; p-O₂NC₆H₄, Me, OH, above 310°, 90, repptd.; p-O₂NC₆H₄, Me, Cl, 184°, 82, PhMe. V were prepared by the following methods: (method A) IV (R₁ = H, R₂ = Me) (10 g.) and 120 ml. alc. NH₃ heated 8 hrs. in a bomb at 160°, the product evaporated to dryness, the residue refluxed with dilute HCl, the solution treated with C, filtered, and the product repptd. with NH₄OH, filtered, and recrystd. gave 6.5 g. V (R₁ = R₄ = R₅ = H, R₂ = Me); (method B) the above IV (5 g.) added to 7 g. BuNH₂, and 120 ml. alc. and the mixture refluxed 7 hrs. gave 3 g. V (R₁ = R₄ = H, R₂ = Me, R₅ = Bu). IV (R₁ = Ph, R₂ = Me) (5 g.) refluxed 40 min. with 8 g. p-ClC₆H₄NH₂ and 75 ml. alc. and the mixture filtered after cooling 3 hrs. in an ice bath gave 6.2 g. crude V (R₁ = Ph, R₂ = Me, R₄ = H, R₅ = p-ClC₆H₄). IV (R₁ = p-ClC₆H₄, R₂ = Me) (9 g.) refluxed on a steam bath to near dryness with 160 ml. alc. containing 10 g. PhCH₂CH₂NH₂ and the residue added to MeOH gave 11 g. V (R₁ = p-ClC₆H₄, R₂ = Me, R₄ = H, R₅ = CH₂CH₂Ph); (method C) IV (R₁ = R₂ = Me) (5.5 g.), 5.5 g. furfurylamine, and 200 ml. alc. heated 8 hrs. on a steam bath, then evaporated, the residue stirred with 30 ml. 10% KOH, the alkaline solution decanted, the sirup refluxed 2 hrs. with 100 ml. C₆H₆, and the solution, filtered and evaporated to dryness gave

4 g. V (R₁ = R₂ = Me, R₄ = H, R₅ = furfuryl as white needles. IV (R₁ = Ph, R₂ = Et) (13 g.) in 150 ml. alc. treated slowly with 13 g. PhCH₂CH₂NH₂ in 50 ml. alc., the mixture refluxed 12 hrs., the solvent removed, and the product treated with C₆H₆ and several drops MeOH, and refrigerated gave 8 g. V (R₁ = Ph, R₂ = Et, R₄ = H, R₅ = CH₂Ph). The following V were prepared by these methods (R₁, R₂, R₄, R₅, m.p., method of preparation, % yield, and recrystn. solvents given): H, Me, H, H, above 300°, A, 73, alc., H₂O; H, Me, H, Me, above 300°, B, 60, alc., H₂O; H, Me, H, Et, 273-4°, B, 56, alc.; H, Me, H, Pr, 220-2°, B, 49.1, alc.; H, Me, H, CH₂Ph, 241°, B, 87.2, alc.; H, Me, H, furfuryl, 243-4°, C, 59, alc.; Me, Me, H, H, 251-2°, A, 90, alc., H₂O; Me, Me, H, Me, 136-8°, B, 77.2, H₂O; Me, Me, H, Et, 131.5-2.0°, C, 66.9, PhMe, C₇H₁₆; Me, Me, H, CH₂Ph, 180-2°, B, 83, alc.; Me, Me, H, furfuryl, 140-1.5°, C, 54.6, alc.; Me, Me, H, o-ClC₆H₄, 223.5-4.0°, B, 60, alc.; Me, Me, H, p-ClC₆H₄, 231.5°, B, 67, alc., H₂O; Me, Me, H, p-MeC₆H₄, 224-5.5°, B, 60, alc.; Me, Me, H, p-MeC₆H₄, 225-7°, B, 74.7, alc.; Me, Me, H, 2,6-Et₂C₆H₃, 218-18.5°, B, 48.5, alc.; Me, Me, H, NH₂, 259-60°, B, 87.3, alc.; Ph, Me, H, H, 287-9°, A, 82.5, alc., H₂O; Ph, Me, H, Me, 162-3°, B, 80.2, alc., H₂O Ph, Me, Me, Me, 117-17.5°, C, 82.5, alc.; Ph, Me, H, Et, 86°, B, 87.2, alc.; Ph, Me, Et, Et, 66-8°, C, 83, alc.; Ph, Me, H, iso-Pr

143-4°, B 86, alc., H₂O; Ph, Me, H, tert-Bu, 175-7°, C, 61, alc., H₂O; Ph, Me, H, CH₂CH₂NET₂, 159-60°, C, 49.1, C₇H₁₆; Ph, Me, CH₂Ph, H, 187-8°, B, 92, alc.; Ph, Me, H, furfuryl, 153-4.5°, C, 56.2, PhMe, C₇H₁₆; Ph, Me, H, Ph, 262-3°, B, 50.5, EtOCH₂CH₂OH; Ph, Me, H, m-BrC₆H₄, 215-17°, B, 68, alc.; Ph, Me, H, o-ClC₆H₄, 175-6°, B, 51.3, alc.; Ph, Me, H, m-ClC₆H₄, 192-3°, B, 90, alc.; Ph, Me, H, p-ClC₆H₄, 226-6.5°, B, 82, alc., H₂O; Ph, Me, H, 2,6-Et₂C₆H₃, 189-90°, B, 71.2, alc.; Ph, Me, H, NH₂, 243-4°, B, 80.1, C₅H₅N; Ph, Me, H, NHPH, 240-1°, B, 47.5, C₅H₅N; Ph, Et, Me, 90.5-1.0°, B, 55.5, alc.; Ph, Et, H, tert-Bu, 148-8.5°, C 73.3, alc. (sublimed); Ph, Et, H, CH₂Ph, 129-9.5°, C, 48.5, C, 48.5, C₆H₆, alc.; Ph, Et, H, o-ClC₆H₄, 168-8.5°, B, 71.5, EtOCH₂CH₂OH; Ph, Et, H, m-ClC₆H₄, 187-9°, B, 74, alc.; Ph, Et, H, p-ClC₆H₄, 208.5-9.5°, B, 87.8, EtOCH₂CH₂OH; Ph, Et, H, o-MeC₆H₄, 175-6°, B, 75.5, alc.; Ph, Et, H, m-MeC₆H₄, 169.5°, B, 58, alc.; Ph, Et, H, p-MeC₆H₄, 199-200°, B, 78.6, alc.; Ph, Et, H, 2,5-Cl₂C₆H₃, 181-3°, B, 42.1, alc.; Ph, Et, H, 2,6-Et₂C₆H₃, 191-1.5°, B, 38, alc.; Ph, Et, H, NH₂, 198-9°, B, 87.5, alc.; p-MeC₆H₄, Me, H, H, 296.5-8.0°, A, 75.7, alc.; p-MeC₆H₄, Me, H, Me, 181-2.5°, B, 86, MeOH, H₂O; p-MeC₆H₄, Me, Me, Me, 149-51°, B, 82.2, alc.; p-MeC₆H₄, Me, H, Et, 144-6°, B, 80, alc., H₂O; p-MeC₆H₄, Me, H, CH₂CH₂NET₂, 165°, C, 62.8, PhMe, C₇H₁₆; p-MeC₆H₄, Me, H, o-ClC₆H₄, 219-21°, B, 76.5, C₅H₅N; p-MeC₆H₄, Me, H, m-BrC₆H₄, 218-20°, B, 63.5, alc.; o-ClC₆H₄, Me, H, H, 294.5-9.5°, A, 71.8, alc.; o-ClC₆H₄, Me, Me, Me, 152-3°, C, 77.7, alc.; o-ClC₆H₄, Me, H, o-ClC₆H₄, 196-8°, B, 63, alc.; p-BrC₆H₄, Me, Et, Et, 123-4°, B, 51.6, EtOCH₂CH₂OH, H₂O; p-ClC₆H₄, Me, H, H, above 300°, A, 36, alc.; p-ClC₆H₄, Me, H, Me, 218-19°, B, 57.2, alc.; H₂O; p-ClC₆H₄, Me, H, iso-PrO(CH₂)₃, 109-10°, B, 51.1, MeOH, H₂O; p-ClC₆H₄, Me, (R₄R₅ =) (CH₂)₅, 127.5-8.5°, B, 61.3, alc., H₂O; p-ClC₆H₄, Me, H, CH₂Ph, 214°, B, 93.3, EtOCH₂CH₂OH; p-ClC₆H₄, Me, H, CH₂CH₂Ph, 175-6°, B, 60.1, alc.; p-ClC₆H₄, Me, H, o-ClC₆H₄, 221-2°, B, 62.0, C₅H₅N, p-ClC₆H₄, Me, H, m-ClC₆H₄, 222-3°, B, 85.5, EtOCH₂CH₂OH; p-ClC₆H₄, Me, H, p-ClC₆H₄, 239-9.5°, B, 88, C₅H₅N; p-ClC₆H₄, Me, H, m-BrC₆H₄, 230-2°, B, 74.2, C₅H₅N; p-ClC₆H₄, Me, H, 2,5-Cl₂C₆H₃, 200°, B, 71.5, EtOCH₂CH₂OH; p-O₂NC₆H₄, Me, H, Me, 248-9°, B, 69, alc.; p-O₂NC₆H₄, Me, Me, Me, 196°, B, 51.2, alc., H₂O; p-O₂NC₆H₄, Me, H, iso-Pr, 190-2°, B, 81.1, alc.; p-O₂NC₆H₄, Me, H, Bu, 147°, B, 66.6, alc.; p-O₂NC₆H₄, Me, (R₄R₅ =) (CH₂)₅, 189-91°, B, 96, C₅H₅N; p-O₂NC₆H₄, Me, H, CH₂CH₂NET₂, 145°, B, 91.7, alc., H₂O; p-O₂NC₆H₄, Me, H, o-ClC₆H₄, 227-8°, B, 43.2, alc.; p-O₂NC₆H₄, Me, H, p-ClC₆H₄, 278°, B, 87, AcOH. The ultraviolet spectra were given for many of the compds. given above. The screening of these compds. against tumors in mice thus far has not revealed any significant antitumor agents in this series.

IT 5394-42-3P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-ethyl-1-phenyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 5394-42-3 CAPLUS
 CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA
 INDEX NAME)

10556224



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS
RECORD (12 CITINGS)